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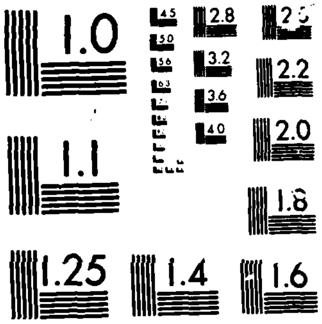

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CRITERIA FOR SELECTION OF GRADED INDEX FILTER MATERIALS BASED ON AN ANALYSIS OF WAVE PROPAGATION IN A PERIODIC MEDIUM

ROGER J. BECKER, Ph.D

UNIVERSITY OF DAYTON RESEARCH INSTITUTE
300 COLLEGE PARK
DAYTON, OHIO 45469-0001

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Donald F. Stevison

DONALD F. STEVISON
Project Engineer

WILLIAM C. KESSLER, CHIEF
Laser Hardened Materials Branch

FOR THE COMMANDER

MERRILL L. MINGES, CHIEF
Electromagnetic Materials Division
Materials Laboratory

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This report includes a survey of the factors affecting the performance of a filter. Although specifically directed at optical filters, most of the discussion is quite general, applying to the propagation of any wave in a medium with a spatially modulated response or susceptance. The intent of this work is to examine the factors affecting filter performance with a view toward perfecting filter design, to gain a deeper understanding of the relationship between rugate index profile parameters and the consequent optical properties, and to guide rugate deposition experiments.

A wide range of systems which are usually treated as unique share important features with optical filters. Examples are acoustic filters, electronic energy bands in solid, lattice dynamics, transmission line theory, and waveguide theory. This report begins to lay the groundwork for development of an optimum transfer function and to determine the appropriate values for the filter parameters.

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DONALD F. STEVISON

22b. TELEPHONE NUMBER *(Include Area Code)*
(513) 255-52110

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FOREWORD

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*of University of Dayton

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CRITERIA FOR SELECTION OF GRADED INDEX FILTER MATERIALS BASED ON AN ANALYSIS OF WAVE PROPAGATION IN A PERIODIC MEDIUM

Roger J. Becker, Ph.D.

University of Dayton
Research Institute
Dayton, Ohio 45469

UNIVERSITY OF DAYTON
RESEARCH INSTITUTE
DAYTON, OHIO 45469

1. INTRODUCTION

This document is a preliminary report on a survey of the factors affecting the performance of a filter. Although specifically directed at optical filters, most of the discussion is quite general, applying to the propagation of any wave in a medium with a spatially modulated response or susceptance. The intent of this work is to examine the factors affecting filter performance with a view toward perfecting filter design. This effort began with a survey of the optical properties of materials which could be used in a filter. The assumption was that ultimate filter performance is primarily limited by materials questions. During this survey the author quickly became aware of the need to develop a rating system for material properties, based on the relationships between filter performance and the susceptance of the various parts of the filter. Thus it became necessary to first establish this relationship, a task which forms the main body of this work.

1.1 Design Needs

The filter design engineer is severely hampered if he does not have the freedom to specify the susceptance (this implies the refractive index) of the medium at a given location. A dielectric can be tailored to an arbitrary specification between the limiting value of the dielectric constants of a given set of materials by making an appropriate solution of these materials. Unfortunately there is no ready formula for the ideal solution (this question is addressed in Paragraph 2.1) and no solution will be perfectly homogeneous. The impact of this fact on wave propagation is discussed in Paragraph 2.2.

Bragg filters are based on the interference effects upon wave propagation due to spatial variations in the susceptance of the medium. Traditional optical filters have modulated the refractive index profile in discrete, discontinuous steps. The index response between these steps is flat. This method achieves great simplicity in both manufacture and design. The motivation for this work is the production of a new type of filter--the graded index filter. We define a graded index filter as one in which the medium susceptance (and therefore the dielectric constant) is smoothly and continuously varying, i.e., one in which there are no sharp discontinuities or flat regions in the susceptance. Currently a sinusoidal modulation is popular in design.

Much of the impetus for the development of graded index filters is based upon the speculation that the freedom to contour the index profile at will should allow the design engineer extra flexibility in the design of filters with ultra narrow stop, or reflectance bands, the location of several such bands at arbitrary frequencies, and the avoidance of absorption and/or scattering associated with material discontinuities. The author has uncovered nothing in this study to support these beliefs. On the contrary, the analysis presented here suggests that details of the modulation profile have little bearing on filter performance in the frequency range for which most simple filters are designed.

Wave propagation in a periodic medium is governed primarily by fundamental considerations without regard to the details of the system in question (some of these fundamental features are discussed in the Appendix). Consequently, a wide range of systems which are usually treated as unique share important features with optical filters. Examples are acoustic filters (mufflers), electronic energy bands in solids, lattice dynamics, transmission line theory, and waveguide theory. Insight to the optical filter problem can be gained by reviewing the large body of work developed in these other related areas. In particular, it is universally found that a periodic modulation of the medium response will produce not just a single stop, or reflectance band, but a series of such bands with increasing frequency. In solid-state band theory, these stop bands are referred to as band gaps. The higher order band structure is related to the details of the modulation profile. In the event a filter is designed for a multi-octave frequency range, the details of the index contour will become important.

1.2 Approach

The analysis adopted in the following review of filter performance is analytic. The philosophy is that an analytic (in contrast to a numerical) approach has advantages for conferring insight on the essential physical parameters that determine filter performance. In the process of pursuing this approach a second goal developed: the application of analysis to optical filter design, especially the design of continuous gradient filters. A general procedure for designing a filter is given in Figure 1.1, which is taken from a reference on the design of filters in transmission lines.[1] This report begins to lay the groundwork for development of an optimum transfer function and a determination of appropriate values for the filter parameters. The author believes that this analysis will answer questions on the effect of discontinuities and of continuously varying susceptibilities on filter performance, and the degree to which an ideal notch filter can be approximated.

An analytic approach has special advantages when a problem becomes complex. An example is the extension of simple, one-dimensional filters with purely real refraction indices to three-

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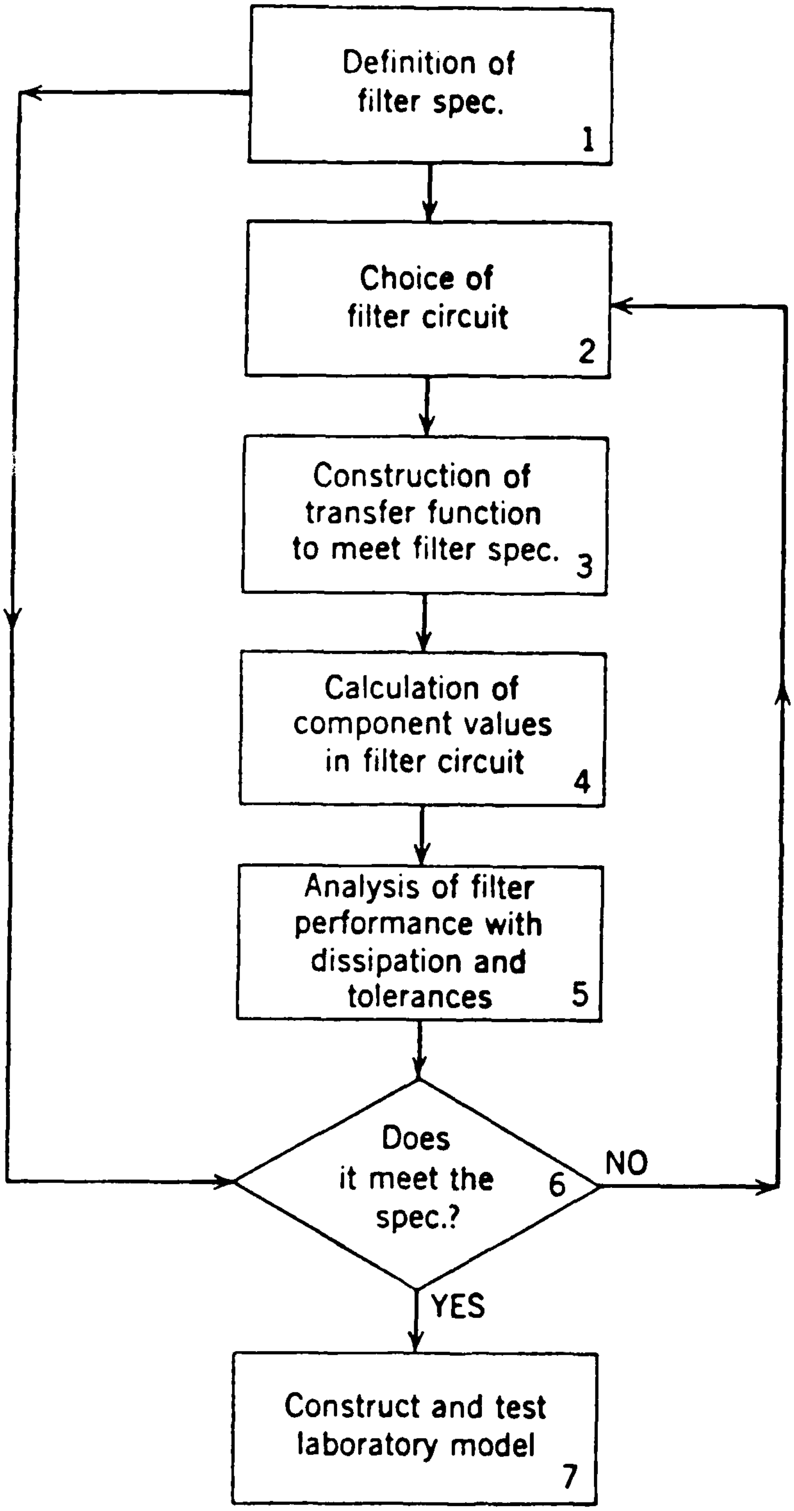

Figure 1. Approach to filter design used in transmission line theory.

dimensional filters with complex susceptibilities. This problem can be handled analytically by a resolvant, or Green's function approach. The Green's function method is a generalization of the concepts addressed in this report.

Section 3 presents an overview of filters, of different means of describing their performance, and of the diverse subjects which share essential features. The critical conclusion of Section 3 is that a complete description of the performance of a filter may be obtained once the wave equation is solved over the fundamental repeat region (unit cell) of the filter cascade. The solution of the wave equation is then discussed in Section 4, with special emphasis on the two cases of special interest, step function and sinusoidal modulation. These two cases are compared, and some general observations are made about the behavior of the solutions, particularly the appearance of stop and pass bands.

Sections 5 and 6 discuss various means by which the solution of the wave equation may be converted to an algebraic problem. Algebraic procedures are especially useful in describing multiple periodic filters, as well as terminations, junctions, and other local departures from the periodic profile. They are a prime analytic tool. The mathematical basis for Section 5 is given in Appendix A.

Several candidates for optical filter materials are discussed in Section 7, largely in terms of crystal structure and lattice parameters, since these must be well matched to obtain a minimal-defect solution. We call attention to the as-yet-little-studied layered materials, in particular the transition metal chalcogenides. Our conclusions and suggestions for future work are given in Section 8. Although this report is largely the result of an extensive literature review, every section contains significant original contributions by the author.

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1. Gabor C. Temes and Sanjit K. Mitra, Modern Filter Theory & Design.

2. PRELIMINARY CONSIDERATIONS ON DIELECTRIC BEHAVIOR

The following three sections will give a mathematical description of light propagation in an ideal medium. In this section we comment on formulas appearing in the literature for tailor-made dielectrics and on the effect of a material's imperfections on its ideal behavior.

2.1 Dielectric Constant of a Mixture

Before we examine how departures from an ideal profile will affect the response of an inhomogeneous medium, we should first obtain some insight into the dielectric behavior of a solution. To our knowledge, this matter has not been adequately explored. The dielectric constant of a material is a macroscopic property with a nonlinear dependence on the molecular (microscopic) polarizability. The reason for this nonlinearity is the depolarizing response to an external field created at any discontinuity in the susceptibility of the medium. Consequently, accurate models of dielectric behavior must take account of the effect of the surrounding medium on the microscopic susceptibility of a material. Unfortunately, this behavior is very complex. We now derive a general result for a multi-component dielectric mixture. The relation of our result to earlier work and suggestions for extensions follow.

We denote the applied electric field, the local effective electric field, and the net polarization field respectively by E, E', and P. We will model the medium by a solution of molecules with ellipsoidal shapes. The polarizability of a molecule of a given species will be denoted α_i. We have

$$E' = E + 4\pi AP \qquad (2.1)$$

and

$$P = \sum_i p_i = E' \sum_i \alpha_i , \tag{2.2}$$

or

$$P = (E + 4\pi AP) \sum_i \alpha_i \quad . \tag{2.3}$$

Here p_i is the induced dipole moment of a molecule of species i, and A is a factor varying from 0 to 1, depending on the shape of the ellipsoid. A = 1/3 for spheres. Our summations are actually double summations, in which we sum over all the molecules of each species, i.e., we use a suppressed notation. We may rewrite Equation (2.3) to obtain

$$\sum_i \alpha_i = P/(E + 4\pi AP), \tag{2.4}$$

and

$$(1 - 4\pi A \sum_i \alpha_i)\, P = E \sum_i \alpha_i \quad . \tag{2.5}$$

We have

$$P = \chi E \quad , \tag{2.6}$$

with the dielectric constant given by

$$\varepsilon = 1 + 4\pi\chi \quad . \tag{2.7}$$

We may obtain our desired relations:

$$\sum_i \alpha_i = \frac{1}{4\pi} \frac{(\varepsilon - 1)}{(1 - A) + A\varepsilon} \tag{2.8}$$

and

$$\varepsilon - 1 = \frac{4\pi \sum_i \alpha_i}{1 - 4\pi A \sum_i \alpha_i} \tag{2.9}$$

or

$$\varepsilon = \frac{1 + 4\pi(1 - A) \sum_i \alpha_i}{1 - 4\pi A \sum_i \alpha_i} \tag{2.10}$$

These relations neglect permanent dipole moments. In fact, most materials of interest in hard filters are polar; nevertheless our neglect of permanent dipole moments remains valid at optical frequencies. In the intermediate infrared region the permanent molecular dipoles can respond to the applied field, so we must make the substitution

$$\alpha_i \rightarrow \alpha_i + \mu_i^2 / (3kT + b\, n_i \mu_i^2) \tag{2.11}$$

for dipoles μ_i of series i with concentration n_i at a temperature T. In Equation (2.11), b is an empirical constant.

We obtain a relation between the macroscopic parameters ε and ε_1 and ε_2 for a two-component solution of molecular densities n_1 and n_2 by an iteration of Equation (2.8):

$$\frac{(n_1 + n_2)(\varepsilon - 1)}{1 - A + A\varepsilon} = \frac{n_1(\varepsilon_1 - 1)}{1 - A + A\varepsilon_1} + \frac{n_2(\varepsilon_2 - 1)}{1 - A + A\varepsilon_2}. \tag{2.12}$$

This yields

$$[(1 - A)(n_1 + n_2) + A(n_1\varepsilon_2 + n_2\varepsilon_1)]\,\varepsilon =$$

$$(n_1 + n_2) A\varepsilon_1\varepsilon_2 + (1 - A)(n_1\varepsilon_1 + n_2\varepsilon_2) , \tag{2.13}$$

which leads to

$$\varepsilon = \frac{n_1 a_1 \varepsilon_1 + n_2 a_2 \varepsilon_2}{n_1 a_1 + n_2 a_2} , \tag{2.14}$$

where

$$a_i = 1/(A\varepsilon_i + 1 - A) \quad . \qquad (2.15)$$

When A = 1/3 and 0 we respectively obtain the relations for the Clausius-Mossotti and "Drude," or more properly, Sellmeier models given by Bottcher[1] and Jacobsson.[2] We note that the simplified form found in Equation (2.14) is only valid if A is the same for both species. It can be extended to include a summation over several species in a solution.

We can extend Equation (2.14) by induction, and give here an illustration of the first step in the induction argument, a three-component solution. We consider the solution to be composed of a two-component solution plus the third component, and use the subscript o to refer to the two-component solution. Then from Equation (2.14) we have

$$\varepsilon = \frac{n_o a_o \varepsilon_o + n_3 a_3 \varepsilon_3}{n_o + n_3 a_3} \quad . \qquad (2.16)$$

Again from Equation (2.14), we rewrite Equation (2.16) as

$$\varepsilon = \frac{(n_1+n_2)\, a_o \dfrac{n_1 a_1 \varepsilon_1 + n_2 a_2 \varepsilon_2}{n_1 a_1 + n_2 a_2} + n_3 a_3 \varepsilon_3}{(n_1+n_2) a_o + n_3 \varepsilon_3} \quad . \qquad (2.17)$$

Now

$$a_o = (A\varepsilon_o + 1 - A)^{-1} \qquad (2.18)$$

or

$$a_o = 1/\left[A \frac{n_1 a_1 \varepsilon_1 + n_2 a_2 \varepsilon_2}{n_1 a_1 + n_2 a_2} + 1 - A\right] \quad . \qquad (2.19)$$

Consequently

$$(n_1 + n_2) a_o = \frac{n_1 + n_2}{A a_1 (\varepsilon_1 - 1)\, n_1 + A a_2 (\varepsilon_2 - 1) n_2} \quad . \qquad (2.20)$$

From Equation (2.15), we see that

$$(n_1 + n_2)\, a_o = n_1 a_1 + n_2 a_2 \quad . \qquad (2.21)$$

Substitution of Equation (2.21) in Equation (2.17) gives

$$\varepsilon = \frac{\sum_1^3 n_i a_i \varepsilon_i}{\sum_1^3 n_i a_i} \quad . \qquad \text{Q.E.D.} \qquad (2.22)$$

Clearly, we may iterate this argument to include any number of species of the same A coefficient.

In general, ε, χ, and α will be complex. Equation (2.14) is valid for complex dielectric constants, as may be seen from its derivation. Part of its utility is that it gives a result for complex dielectric constants without reference to the details of the microscopic polarizability. From our derivation, we see that Equation (2.14) should also include a reasonable amount of dispersion, by letting $\varepsilon \rightarrow \varepsilon(\omega)$.

In Equation (2.14) we recover the value for a pure material if either n_1 or $n_2 \rightarrow 0$, as we should. In a mixture ε is reduced from a value given by a linear interpolation between ε_1 and ε_2 for $A \neq 0$ due to the interaction between molecules. To see this, consider a solution when $n_1 = n_2$. Then we find

$$\varepsilon = \frac{2A\varepsilon_1\varepsilon_2 + (1 - A)\,(\varepsilon_1 + \varepsilon_2)}{2(1 - A) + A(\varepsilon_1 + \varepsilon_2)} \quad . \qquad (2.23)$$

Comparing this with $(\varepsilon_1 + \varepsilon_2)/2$ we obtain the variation in ε from its value found from a linear interpolation, $\delta\varepsilon$:

$$\delta\varepsilon = \frac{A(\varepsilon_1 - \varepsilon_2)^2}{4[2(1 - A) + A(\varepsilon_1 + \varepsilon_2)]} \quad . \qquad (2.24)$$

We see that $\delta\varepsilon$ will increase with both A and $\varepsilon_2 - \varepsilon_1$. This is consistent with experiment and the discussion given by Jacobsson.[2] However, part of Jacobsson's treatment contains errors, since it is based on a faulty premise which we now describe.

If an ellipsoid with dielectric constant ε_2 is embedded in a uniform medium of dielectric constant ε_1 then a net simple dipole field proportional to $\varepsilon_2 - \varepsilon_1$ will be added to the effective field that would occur in the absence of the ellipsoid.[3] Using this result, Polder and Van Santen[4] obtained the effective dielectric constant for a dilute suspension of such spheres.

$$\varepsilon = \varepsilon_1 + C\varepsilon_1(\varepsilon_2 - \varepsilon_1)/[A\varepsilon_2 + (1 - A)\varepsilon_1] \quad , \qquad (2.25)$$

where C is the volume concentration of the ellipsoids. This result is readily extended to include ellipsoids of varying dielectric constant and shape. A similar result is found by Landau and Lifshitz for spheres.[5] However, these authors were mindful of the difference between a dilute suspension and a strong solution, noting that Equation (2.25) can only be taken as an approximation for a solution at low concentrations. We may attempt to extend Equation (2.25) by using the approximation

$$\varepsilon = \varepsilon_1 + C\varepsilon N\varepsilon_2 - \varepsilon_1)/[A\varepsilon_2 + (1 - A)\varepsilon] \quad , \qquad (2.26)$$

as Polder and Van Santen in fact did, but this formula also breaks down as C increases, as may be seen by comparison with Equation (2.12) using $C = n_2/(n_1 + n_2)$. Jacobsson ignores this limitation.

Equation (2.26) is a macroscopic result. It pertains to particles in a homogeneous background. We may well treat the interaction between a molecule and distant molecules by an average field,[6] but must be careful about our treatment of local interactions. Jackson,[6] shows that the Clausius-Mossotti result (A = 1/3) should work well for distant interactions, with local fields accounted for by a perturbation parameter s,

$$A = 1/3 + s \quad . \tag{2.27}$$

For symmetrical systems, such as cubic crystals and pure amorphous materials, the various contributions which include s cancel. This is why the Clausius-Mossotti equation is so useful.

Departures observed from the values predicted using $A = 1/3$ are observed in bicomponent films.[2] This may be due to a lack of local isotropy, but could well be due to local departures from stoichiometry and voids. It is impossible to say without a thorough characterization of the films. As can be seen from Equation (2.25), voids can have a dramatic impact on the dielectric constant.

The derivation leading to Equation (2.8) is inexact. A more accurate formulation can be obtained following the Onsager development for spheres.[1] In fact, we could use a statistical treatment.[1] In our treatment we have swept statistical variations in the local dielectric environment of a molecule under the rug, burying the resulting parameter s in our parameter A. In other words, our treatment is intended only as a model that will include the effect of an inhomogeneous local environment. However, we believe it gives a better picture than an uncritical use of Equation (2.26). It cannot readily be extended to include solutions of materials with different values for A. However, Equation (2.8) should be adequate for our purposes. In fact, until it is established that departures from the Clausius-Mossotti relation are in fact due to molecular shape factors rather than film preparation, we may well choose $A = 1/3$. For design purposes it is probably best to use empirical values for the dielectric constants of mixtures, since they are so heavily dependent on fabrication processes.

2.2 Rayleigh Scattering from Inhomogeneities in ε

Local variations from the desired dielectric coefficient will mar its performance. We are concerned here with random, local imperfections, rather than regular one-dimension discontinuities in the dielectric profile. These imperfections will include voids, departures from stoichiometry due to lack of control during fabrication, departures from stoichiometry due to compositional segregation following fabrication, surface roughness at film interfaces, impurities, density fluctuations in amorphous films, the occurrence of microcrystals in an amorphous matrix, and polycrystalline films containing more than one phase, or randomly oriented crystals with anisotropic refractive indices. We assume that all these imperfections, if they occur, will be small in size. This will allow us to make a Rayleigh scattering approximation. Consequently we will not need to consider the shape of the scattering centers, although except for the case of voids we may easily extend our discussion to include centers of any shape.[7] Similarly, we will ignore gradations in the index profile of imperfections, and model them by spheres of uniform dielectric strength. A more accurate description will add little to our conclusions at the cost of great complications, since we can account for most effects by choosing an effective radius, a, for the scattering centers. We will also neglect coherence effects. We denote the scattering cross section by σ_s and the absorption cross section by σ_a. We let the local dielectric constant of the medium be ε_m, and that of the imperfection be ε_i. We have

$$\sigma_s = \frac{8\pi}{3} k^4 \left[\frac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}\right]^2 a^6 \qquad (2.28)$$

and

$$\sigma_a = 4\pi k \; I_m\left[\frac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}\right] a^3 \qquad (2.29)$$

$$\simeq 4\pi k \left[\frac{\varepsilon_i'' - \varepsilon_m''}{\varepsilon_i + 2\varepsilon_m} \right] a^3 \quad , \tag{2.30}$$

assuming that the imaginary part of ε, ε'' is small compared to its real part, ε'. Here

$$k = 2\pi\sqrt{\varepsilon_m}/\lambda_0 , \tag{2.31}$$

is the wave vector in the medium surrounding the scattering center corresponding to a freespace wavelength λ_0. We see that

$$\frac{\sigma_a}{\sigma_s} \simeq \frac{3}{2} \frac{(\varepsilon_i + 2\varepsilon_m)}{(ka)^3} \frac{(\varepsilon_i'' - \varepsilon_m'')}{(\varepsilon_i - \varepsilon_m)^2} \quad . \tag{2.32}$$

Since we are considering a regime in which $ka \ll 1$, absorption will be important, and in fact will probably dominate. An exception to this rule will again be the case of voids.

From Equation (2.28) we see that scattering will be far more severe in the optical region than in the infrared. Absorption will also be more severe, although not proportionately. We will assume that the density of scattering centers is sufficiently low, so that we may restrict ourselves to single particle scattering. The intensity at a depth z in the filter, I(z), will be given by

$$I(z) = I_0 \exp\left[\int dz \; n(z) \; \sigma_e(z) , \right. \tag{2.33}$$

where I_0 is the input intensity and

$$\sigma_e = \sigma_s + \sigma_a \quad . \tag{2.34}$$

We see from Equation (2.29) that the total absorption per unit length due to a given type of imperfection is proportional to the fractional volume of scattering centers in the material. Thus for small centers the relative importance of a given type of imperfection is roughly proportional to $C\ (\varepsilon_i'' - \varepsilon_m'')$, where C is the fractional volume of that type of impurity.

We now present models for the dielectric behavior of several imperfections. Voids will have the strongest scattering for a given size scattering center, but will not contribute to absorption. We have

$$\varepsilon_i' = 1 \quad , \quad \varepsilon_i'' = 0 \quad . \tag{2.35}$$

A tendency towards separation or decomposition of the solution will drive both ε_1 and ε_m toward ε_1 or ε_2. In the limit of complete separation we will have

$$\varepsilon_i \rightarrow \varepsilon_2 \ , \quad \varepsilon_m \rightarrow \varepsilon_1 \quad . \tag{2.36}$$

We may treat a partial decomposition in the same manner as a variation in stoichiometry. Let

$$\varepsilon \simeq n_1 \varepsilon_1 + n_2 \varepsilon_2 \quad . \tag{2.37}$$

Then for a fractional change δ in composition we will have

$$\varepsilon \simeq \left(n_1 \varepsilon_1 + n_2 \varepsilon_2\right) + \delta\left(\varepsilon_1 - \varepsilon_2\right) \quad , \tag{2.38}$$

so that

$$\varepsilon_i \simeq \delta\left(\varepsilon_1 - \varepsilon_2\right) \tag{2.39}$$

and

$$\varepsilon_i'' - \varepsilon_m'' \simeq \delta\left(\varepsilon_1'' - \varepsilon_2''\right) \quad . \tag{2.40}$$

We expect δ to be on the order of a few percent.

If the dielectric constant changes due to a change in phase, or in the case of an anisotropic medium, to a change in orientation, we model it as

$$\varepsilon_i = \varepsilon_m(1 \pm \Delta) \quad , \tag{2.41}$$

so that

$$\varepsilon_i'' - \varepsilon_m'' \simeq \pm \Delta\varepsilon_m'' \quad . \tag{2.42}$$

We expect that Δ may be on the order of several percent. There may also be a small change in the dielectric constant at the boundaries of grains in polycrystaline material or at film interfaces. Here also we expect a relations like those of Equations (2.41) and (2.42), with the fractional volume of scattering centers proportional to the surface to volume ratio of the grains or films.

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3. WAVE PROPAGATION IN A PERIODIC STRUCTURE

All periodic structures act as filters to waves passing through them, i.e., they have pass and stop bands. The problem we wish to solve, the optical filtering properties of a material with a modulated index of refraction, is very similar to other problems in acoustics,[1-5] electrical transmission lines,[6,7] microwave waveguides,[8-16] solid-state band theory,[17-40] and lattice dynamics.[41-43] We can gain a great deal of insight from the work done in these related areas. The first thing that becomes apparent in comparisons with these other systems is that the stop and pass bands do not depend greatly on the specific nature of the wave in question; rather they simply arise from the regular variation of the response of the transmitting medium to the disturbance of the wave.

Procedures for analytic treatment of problems of this kind are well developed. We now summarize them and give examples. We will then comment on the possibilities for inversion, investigating high-order band behavior, two and three dimensional calculations, and the similarities and differences between the response of filters with slightly different index profiles.

3.1 Graphic Displays of Performance

The result of a calculation will be a curve. It may be a transmission or reflection coefficient curve,[44,45] displaying the transmission coefficient, T, or reflection coefficient, R, versus the incident wavenumber, k_o. It may also be a dispersion curve,[46-50] displaying the real part of the frequency of the incident wave, ω, (which is equivalent to k_o) versus the wavenumber in the medium, k. These two types of curves contain similar information, since attenuated transmission is accounted for by a complex value for ω, and we can easily plot the imaginary part of ω as well as its real part. When the attenuation is small, there are some advantages to using the dispersion curves instead of reflection curves. The dispersion curves give a clear picture of the pass and stop bands above the fundamental bands. They give a good picture of behavior in three-dimensional systems, are very useful in analyzing mode coupling and the density of states, or channel carrying capacity in a given frequency range, $\Delta\omega$. Consequently dispersion curves are commonly used in solid-state physics and waveguide transmission problems. Apparently this type of analysis has been relatively little used in optics. Optical problems have more commonly been expressed in terms of reflection and transmission coefficients, which have advantages when absorption by the medium is large or when the ratio of the filter thickness, t, to the length characterizing its periodicity (unit cell length), d, is small. Since dispersion curves are useful in obtaining physical insight, we will refer to dispersion curves in most of our discussion.

There are two basic starting points for solving wave transmission problems. The first is a direct solution of the partial differential equation (PDE) for the wave amplitude and phase, ψ. The second is a conversion from a PDE to a difference equation. The difference equation approach is most useful when the index modulation is large over short, well separated regions (tight-binding approximation) or when the modulation is small (nearly free case). In the latter case the difference equation is obtained by a Fourier transformation of the PDE. Of course, the direct solution of the PDE is most useful when the index modulation over a given interval has a behavior close to that in which solutions are known. Perturbation theory may be used with either approach.

Each type of analysis is most useful when expressions for the dispersion/attenuation or reflection/transmission curves are given in terms of the functional form of the index modulation.

However, a good qualitative understanding of a problem is often possible in terms of integrals which may be obtained numerically for specific instances. Figure 3.1 shows the relationships between various functions commonly used in different approaches to the problem.

The solution to the wave equation and its derivative may be thought of as a vector, so that the quantity relating the input and output values of this vector is a matrix. In an optics problem we actually need to know four functions to completely specify one of these vectors, (e.g., for propagation in the x direction we need to know E_x, E_y, H_x, and H_y); so that in general, we need a four-by-four matrix to describe the medium. However, we usually assume a scalor behavior for the dielectric, reducing our four-by-four matrix to two two-by-two matrices, one for TE waves, and one for TM waves. Once we have obtained the matrix coefficients for ψ and ψ' the problem is essentially solved.

3.2 Relationships Between Two Different Approaches

Since the medium is periodic, the dispersion curve is given by an expression of the form[48]

$$\cos kd = \mathrm{Tr}\,[A] \quad , \tag{3.1}$$

where A is a transfer matrix. The elements of A will be functions of the frequency of the incident wave, ω, and the angle of incidence of the incoming wave with respect to the filter. Alternatively we may find the input impedance z_i and characteristic impedance, z_c (or their corresponding admittances) from the elements b_{ij} of A, from relations of the form,[49]

$$z_i = \frac{a_{22}\, z_L - a_{12}}{a_{11} - a_{21}\, z_L} \tag{3.2}$$

and

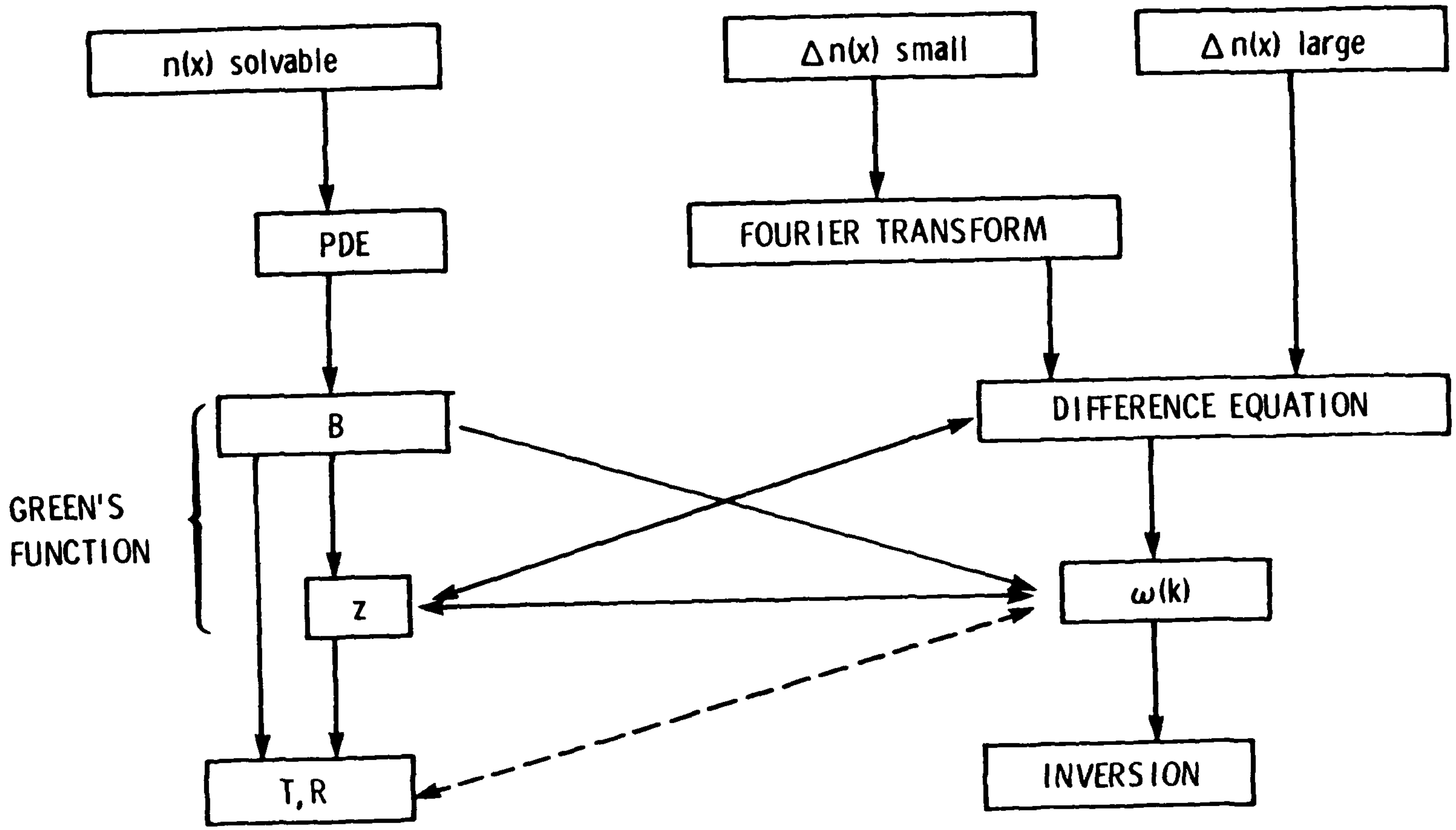


Figure 2. Relationship between various functions in treatments of wave propagation.

$$z_c = [a_{11} - a_{22} \pm i \sqrt{4 - (a_{11} + a_{22})^2}]/2a_{21} \quad . \qquad (3.3)$$

In Equation (3.2) z_i is the load impedance. We see from Equation (3.2) that the impedance concept may be used to describe the effect of terminations, junctions, and local perturbations. However, these quantities can also be described by the difference equation approach. The impedance concept is most useful when the dielectric is a scalar (resulting in two-by-two A matrices) and the problem is one dimensional. More general problems can be expressed in terms of Green's functions, which are closely related to A, z_i, and z_c.

From Equations (3.1) (3.3) we see that we may obtain the dispersion relation in terms of the system impedance. If the system is viewed as a one-dimensional transmission line, we have impedances z_{11}, z_{22}, and z_{12} (see Figure 3.2), with[49]

$$a_{11} = z_{22} / z_{12} \quad , \qquad (3.4)$$

$$a_{22} = z_{11} / z_{12} \quad , \qquad (3.5)$$

$$a_{12} = (z_{12}^2 - z_{11} z_{12})/z_{12} \quad , \qquad (3.6)$$

$$a_{21} = -1/z_{12} , \qquad (3.7)$$

and

$$\cosh kd = (z_{11} + z_{22})/2z_{12} \; , \qquad (3.8)$$

$$z_c = \frac{1}{2} (z_{11} - z_{22}) + z_{12} \sinh kd \quad . \qquad (3.9)$$

The reflection and transmission coefficients may be obtained directly from A, or from Z_{in}. We have[49,50]

$$R_1 = a_{21} / a_{22} \quad , \qquad (3.10)$$

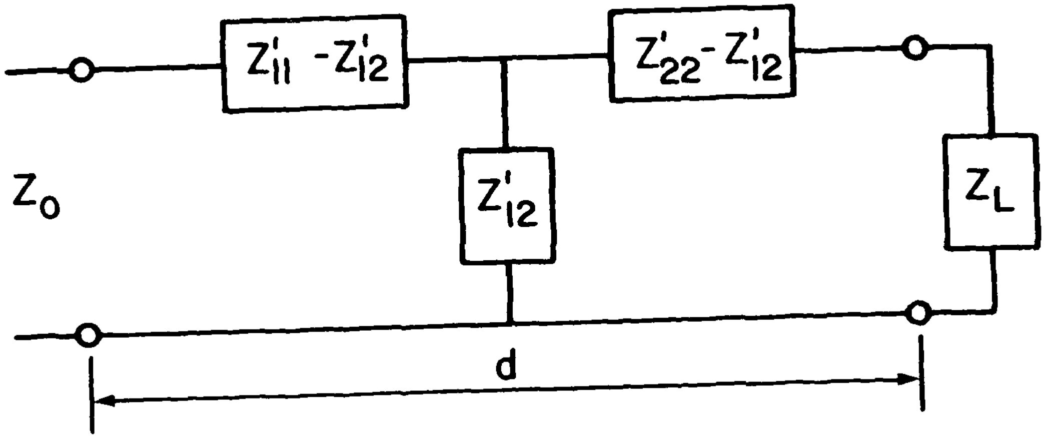


Figure 3. Impedence repeat unit for a transmission line.

$$R_2 = a_{12} / a_{22} \quad , \tag{3.11}$$

and

$$T_{12} = T_{21} = 1/a_{22} \quad ,$$

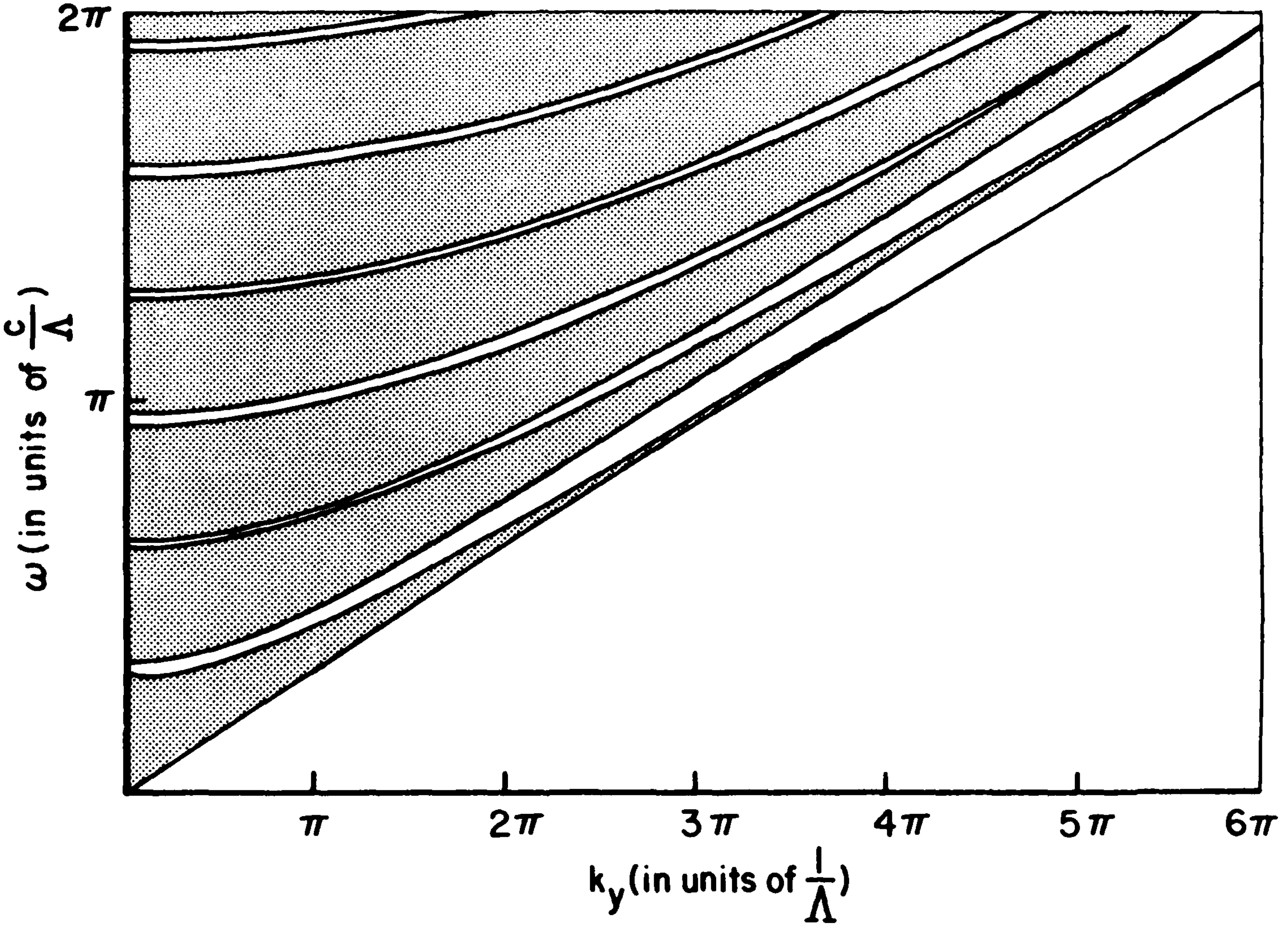
for reflection on the left, R_1, reflection on the right, R_2, and transmission T_{12} or T_{21}. Of course, we will also have[50]

$$R = \frac{z_o - z_i}{z_o + z_i} \quad , \tag{3.12}$$

if the filter is approached via an impedance z_o.

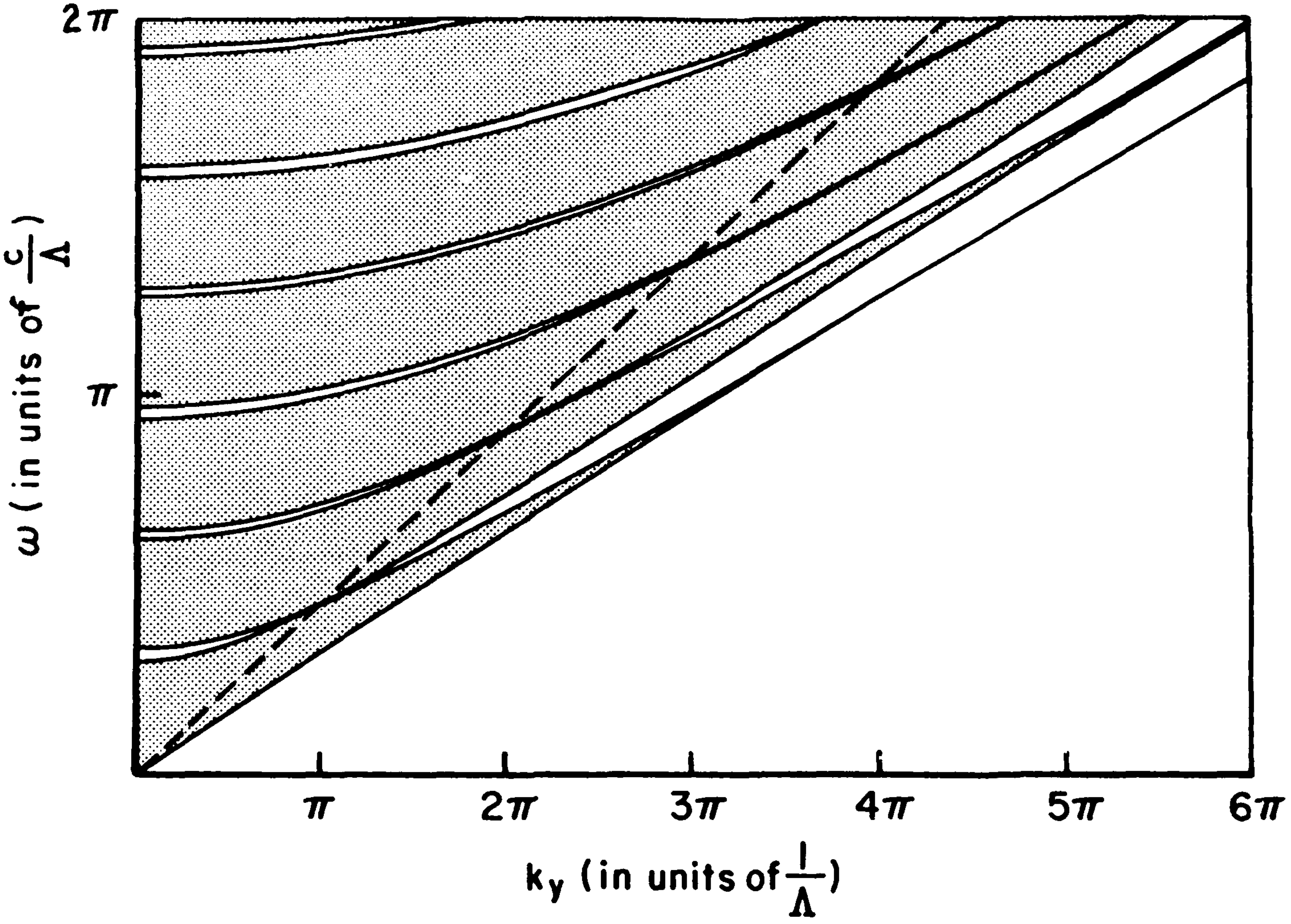
The dispersion curve can also be found from a knowledge of either B or z. This is especially true if A is symmetric, in which case $a_{11} = a_{22}$, and/or an absorption may be neglected, which implies that $\det[A] = 1$. Since the stop and pass band edges occur at $\cos kd = 1$, in the case in which absorption may be neglected, the dispersion curve gives the filtering behavior for a given form for the modulation profile. This provides an understanding of the inverted problem, the specifications required on the modulation potential to obtain a set of predetermined band edges. Similar comments apply to the reflection and transmission curves, provided again that we have expressions in terms of functions, rather than constants. The required expressions will become unwieldy if the solution for ψ within the unit cell of length d cannot be expressed in a compact form. Nevertheless, we know enough from earlier work to say a good deal about the behavior of the dispersion curve resulting from a given modulation profile.

For example, Yeh, Yariv, and Hong[51] have studied light propagation in a filter with a step function (Kronig-Penney) modulation. The results of their calculations are shown in Figures 3.3 to 3.7. In Figures 3.3 and 3.4 the pass and stop bands are plotted as a function of the angle of incidence, θ, with



TE waves (**E** perpendicular to the direction of periodicity): band structure in the ωk_y plane. The dark zones are the allowed bands.

Figure 4. Stop bands as a function of the angle of incidence for a TE wave in a square- well stack.



TM waves (H perpendicular to the direction of periodicity): band structure in the ωk_y plane. The dashed line is $k_y = (\omega/c)n_2 \sin\theta_B$. The dark zones are the allowed bands.

Figure 5. Stop bands as a function of the angle of incidence for a TM wavw in a square-well stack.

$$\beta = k \sin\theta \quad . \tag{3.13}$$

The case studied in Reference 51 dealt only with small modulations, so the stop bands are narrow compared to the pass bands. We see that at low angles of incidence the band edges are insensitive to the angle of incidence. This insensitivity extends to larger angles as the depth of modulation increases. From Figures 3.6 and 3.7 we see that the reflectivity curve corresponds closely to the locations of the stop bands up to fairly high angles of incidence (in this case 40°). In Reference 51 it is shown that the dispersion curve (Figure 3.5) dominates the reflectivity curve at low to moderate angles of incidence. For TM waves the stop bands narrow as they approach the Bragg angle, disappearing altogether at the Bragg angle (Figure 3.7). We note that Figure 3.5 shows how attenuation in the stop bands may be incorporated into a dispersion curve.

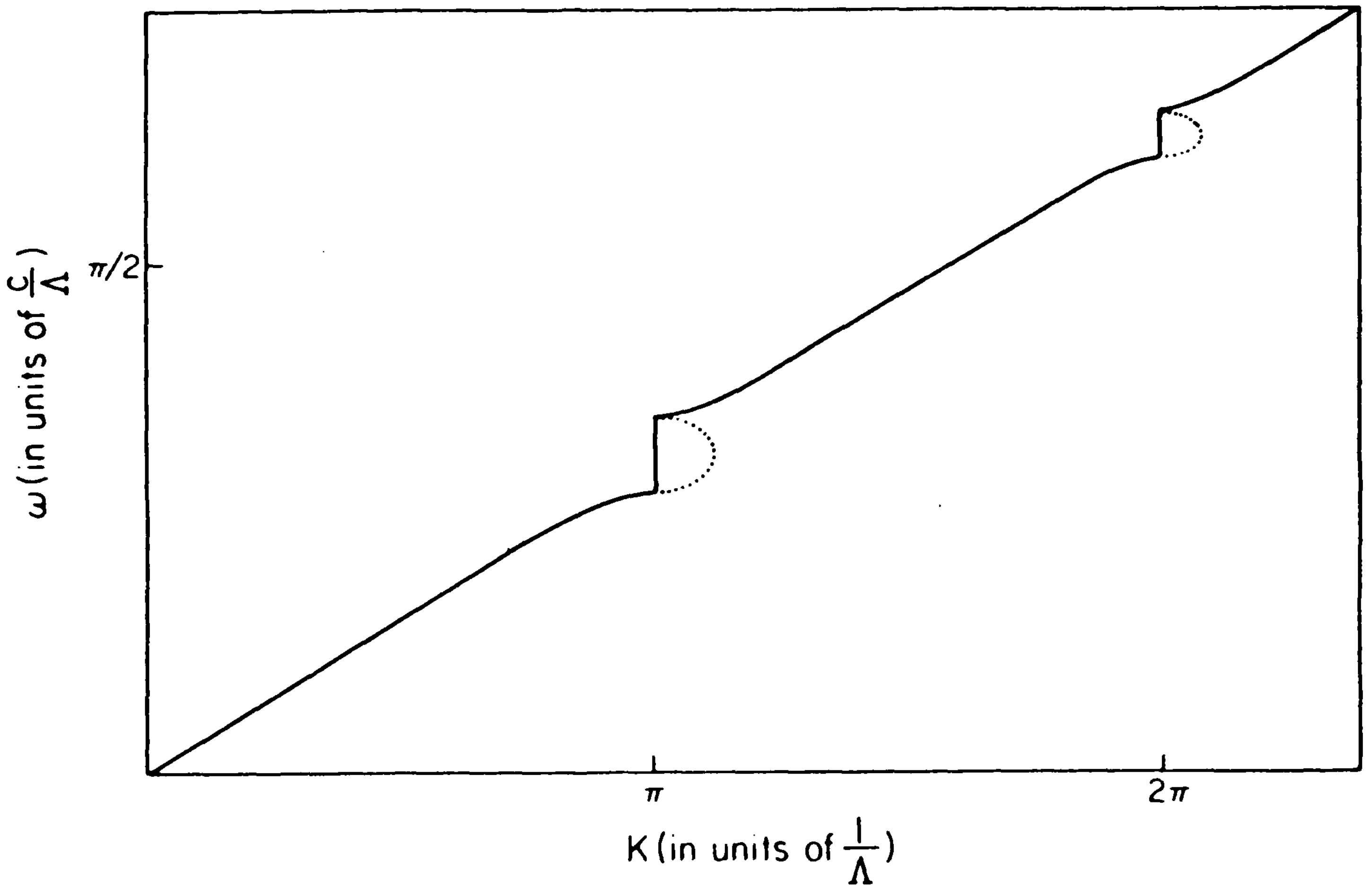
3.3 The Transfer Matrix

Once we have a solution for ψ, we may obtain the matrix elements of B immediately.[52] A second order PDE will have two independent solutions. Let these be ϕ_1 and ϕ_2, and let

$$\psi = c_1\phi_1 + c_2\phi_2 \quad . \tag{3.14}$$

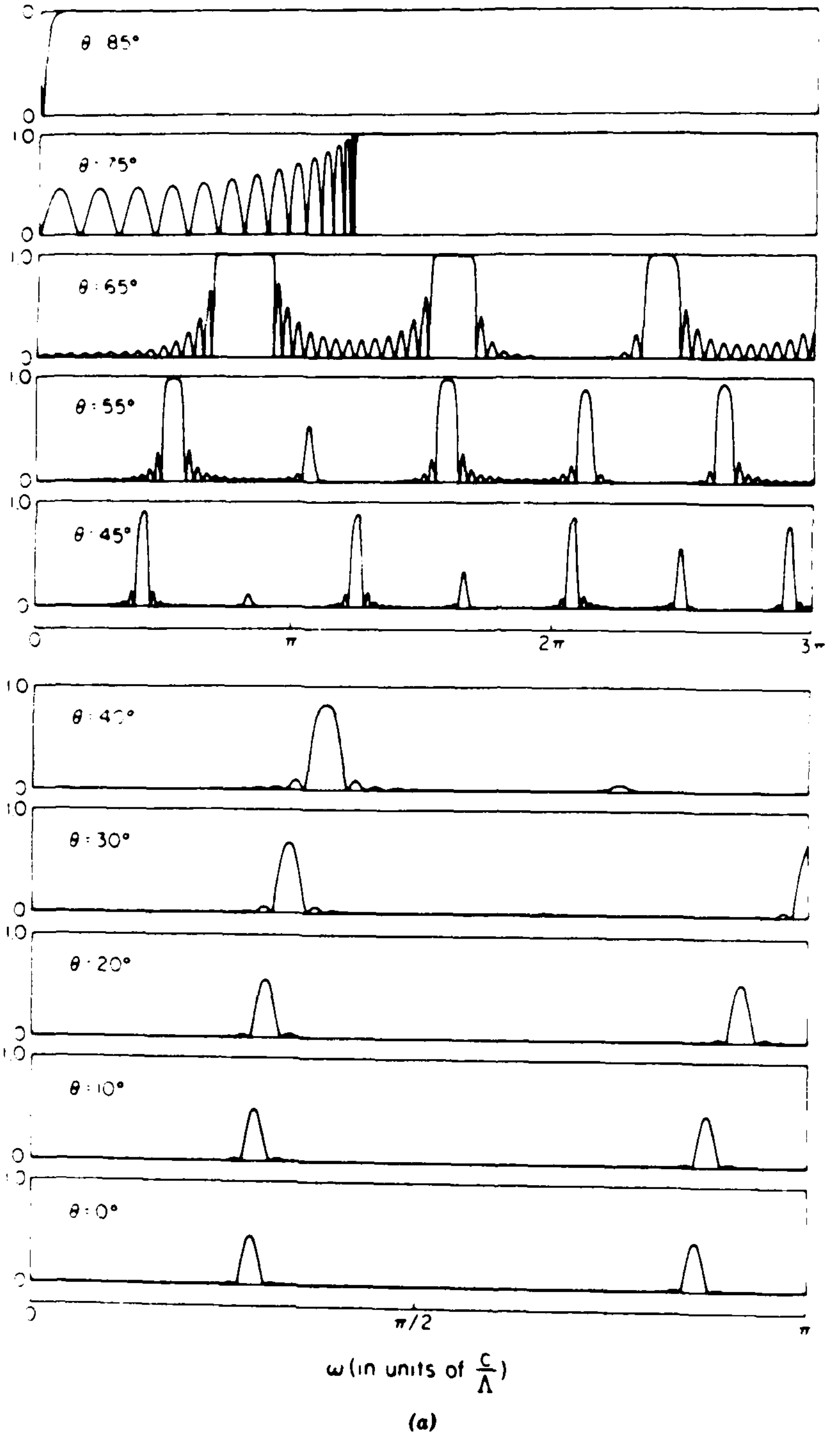
Then

$$\psi' = c_1\phi_1' + c_2\phi_2' \quad . \tag{3.15}$$



The dispersion relation between ω and K when $k_y = 0$ (normal incidence). The dotted curves give the imaginary part of K in arbitrary units.

Figure 6. Dispersion curve as for a periodic square-well stack with low modulation.



Reflectivity spectrum of a 15-period Bragg reflector for (*a*) TE waves and (*b*) TM waves at various angle of incidence. The indices of refraction of the layers are taken as $n_1 = 3.4$ and $n_2 = 3.6$, and the layer thicknesses are such that $a = b = \frac{1}{2}\Lambda$. The Brewster angle is $\theta_B = 46.6°$

Figure 7. Reflectivity as a function of incidence angle for a TE wave in a square-well stack.

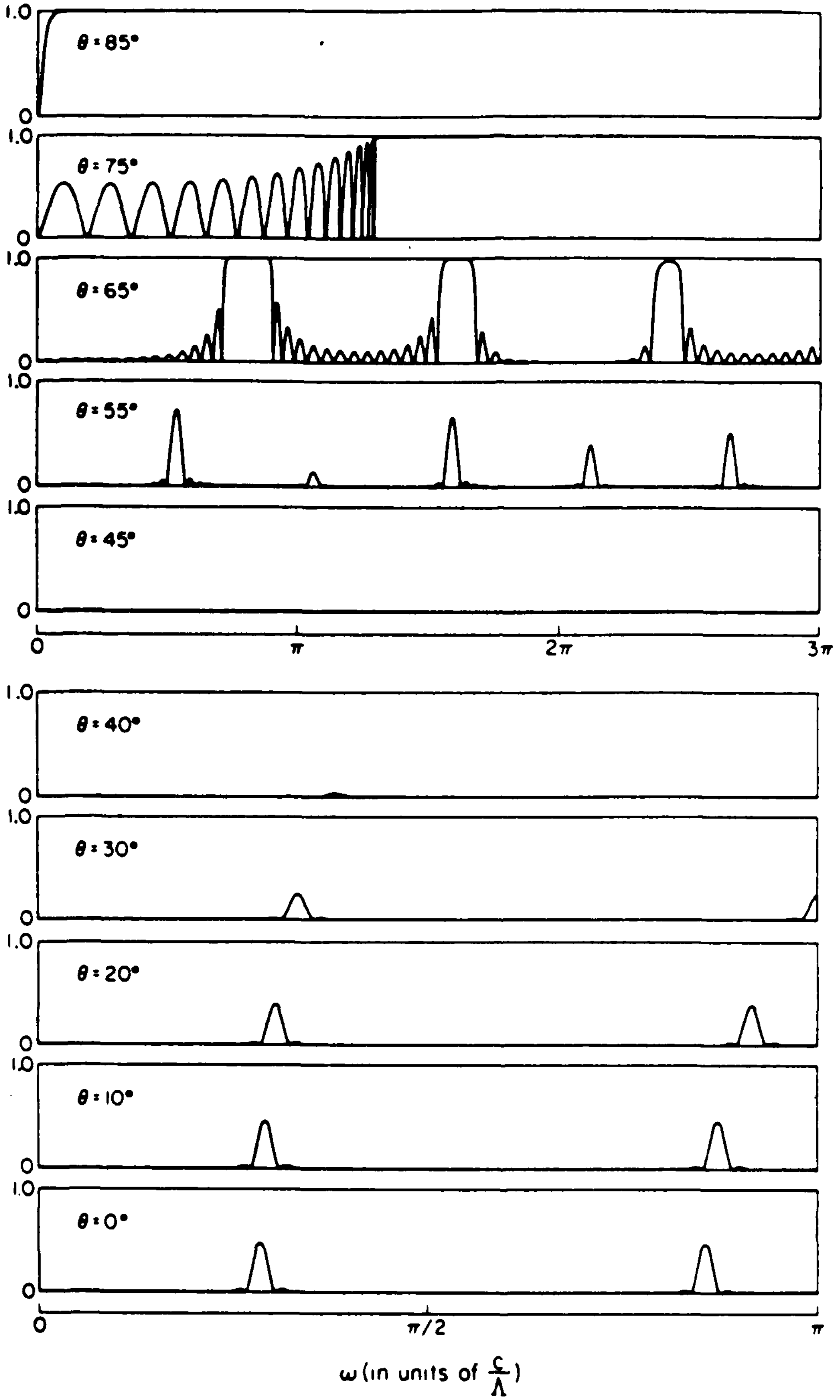


Figure 8 . Reflectivity as a function of incidence angle for a TM wave in a square-well stack.

Solving for c_1 and c_2 we find we can write

$$\begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix} = \begin{bmatrix} B \end{bmatrix} \begin{bmatrix} \psi(x') \\ \psi'(x') \end{bmatrix} , \qquad (3.16)$$

with

$$b_{11} = [\phi_1(x)\phi_2'(x') - \phi_2(x)\phi_1'(x')]/D , \qquad (3.17)$$

$$b_{12} = [\phi_2(x)\phi_1(x') - \phi_1(x)\phi_2(x')]/D , \qquad (3.18)$$

$$b_{21} = [\phi_1'(x)\phi_2'(x') - \phi_2'(x)\phi_1'(x')]/D , \qquad (3.19)$$

and

$$b_{22} = \phi_2'(x)\phi_1(x') - \phi_1'(x)\phi_2(x')]/D , \qquad (3.20)$$

where

$$D = \begin{vmatrix} \phi_1(x) & \phi_2(x) \\ \phi_1'(x) & \phi_2'(x) \end{vmatrix} . \qquad (3.21)$$

We see that

$$b_{11} = -\partial b_{12}/\partial x' \qquad (3.22)$$

$$b_{22} = \partial b_{12}/\partial x , \qquad (3.23)$$

$$b_{21} = \partial b_{11}/\partial x = \partial b_{22}/\partial x' = \partial^2 b_{12}/\partial x \partial x' , \qquad (3.24)$$

and

$$\partial b_{11}/\partial x = \partial b_{22}/\partial x' . \qquad (3.25)$$

Usually we have

$$b_{22} = b_{11}^* . \qquad (3.26)$$

We note that using Equation (3.1), we have

$$\cos kd = [\phi_1(x)\phi_2'(x') - \phi_2(x)\phi_1'(x') + \phi_2'(x)\phi_1(x') - \phi_1'(x)\phi_2(x')]/2D \quad . \tag{3.27}$$

The expression of the matrix elements in terms of x and x' highlights their connection with Green's functions. Often we can reduce these expressions to expressions in terms of one or more distances between x and x'.

For example, for a simple step function modulation with characteristic distances a and b,

$$a + b = d \quad , \tag{3.28}$$

we have[49,53,54]

$$B(x,x') = \begin{bmatrix} G(a,b) & H(a,b) \\ G'(a,b) & H'(a,b) \end{bmatrix} \tag{3.29}$$

3.4 Constant Index

We now illustrate how this may be done, using as an example the solution to the equations

$$d^2\psi/dx^2 + k^2\psi = 0 \quad . \tag{3.30}$$

The solutions are

$$\phi_1 = \cos kx \tag{3.31}$$

and

$$\phi_2 = \sin kx \quad . \tag{3.32}$$

We let

$$x' = x-a \quad , \tag{3.33}$$

and find

$$D = k[\cos^2 kx + \sin^2 kx] = k \quad , \tag{3.34}$$

$$b_{12} = [\sin kx \cos k(x-a) - \cos ka \sin k(x-a)]/k$$

$$= k^{-1} \sin ka \quad , \tag{3.35}$$

$$b_{11} = [k\cos kx \cos k(x-a) + k\sin kx \sin k(x-a)]/k$$

$$= \cos ka \tag{3.36}$$

$$b_{21} = [-k^2 \sin kx \cos k(x-a) + k^2 \cos kx \sin k(x-a)]/k$$

$$= -k\sin ka \tag{3.37}$$

$$b_{22} = [k\cos kx \cos k(x-a) + k\sin kx \sin k(x-a)]/k$$

$$= \cos ka \quad . \tag{3.38}$$

With the identifications

$$G(a) = \cos ka \quad , \tag{3.39}$$

$$H(a) = k^{-1} \sin ka \quad , \tag{3.40}$$

we obtain the form of Equation (3.29).

Expressions for the transfer matrix B in literature give the functions G and H of Equation (3.29) in terms of the unit cell distance d:

$$G(a,b) = G\,(a + b) = G(d) \quad , \tag{3.41}$$

$$H(a,b) = H\,(a + b) = H(d) \quad . \tag{3.42}$$

A comparison of Equations (3.29) and (3.16-3.20) raises the question as to whether the matrix element in Equations

(3.17)-(3.20) can be expressed in terms of d. We are also interested in the connection, if any, between the G and H functions or equivalently, between b_{11} and b_{22}. If such a connection exists, we may solve for the B matrix elements, given the dispersion relation. This would be a great help, since we can often obtain the form for the dispersion relation directly, without first finding the form for B, as we will show in Section 5. This could be one step in an inversion process.

Equations (3.22)-(3.26) suggest a means of answering both of these questions. We may rewrite the relations, Equations (3.17)-(3.20) in terms of the difference between x and x':

$$x - x' = r \quad . \tag{3.43}$$

Usually we will choose r = d. From the definition, Equation (3.43), we obtain

$$\partial r/\partial x = 1 \quad , \quad \partial r/\partial x' = -1 \quad . \tag{3.44}$$

We write

$$d\phi/dr = \phi' \quad , \tag{3.45}$$

and see that

$$\frac{\partial \phi}{\partial x} = \frac{d\phi}{dr}\frac{\partial r}{\partial x} = \phi' \tag{3.46}$$

and

$$\frac{\partial \phi}{\partial x'} = \frac{d\phi}{dr}\frac{\partial r}{\partial x'} = -\phi' \quad . \tag{3.47}$$

Also,

$$\frac{\partial^2 \phi}{\partial x \partial x'} = \frac{d^2 \phi}{dr^2}\frac{\partial^2 r}{\partial x \partial x'} = -\phi'' \quad . \tag{3.48}$$

It seems then, that we may write

$$B = \begin{bmatrix} b' & b \\ -b'' & b' \end{bmatrix} , \tag{3.49}$$

$$\text{i.e., } G \sim H' . \tag{3.50}$$

From Equation (3.49), it appears that we may write Equation (3.1) or Equation (3.27) as

$$2\ b' = \cos kd . \tag{3.51}$$

Consequently, if we have a dispersion relation of the form

$$2\ g(d) = \cos kd , \tag{3.52}$$

we may write

$$b = \int g , \tag{3.53}$$

$$B = \begin{bmatrix} g & \int g \\ -g' & g \end{bmatrix} . \tag{3.54}$$

We see then that the central problem is to solve the PDE equation for ψ. We now discuss means of obtaining this solution further, and give pertinent examples in which the solutions have been obtained.

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4. SOLUTION OF THE WAVE EQUATION

We will make some simplifications in our discussion, mostly for the sake of clarity. We will confine most of our remarks to the one-dimensional problem. We will also deal in general with real refraction indices and infinitely long systems. All of these simplifications can easily be extended to treat a more general case. We will also confine our discussion to systems that are strictly periodic with period d. This is an important boundary condition. From the discussion that follows, we will see that it will not seriously limit the performance of our filter.

We seek to solve equations of the form[1]

$$\frac{d^2U}{dx^2} + k_o^2(n^2(x) - s^2)U = \frac{d\ln\varepsilon}{dx}\frac{dU}{dx} \tag{4.1}$$

and

$$\frac{d^2V}{dx^2} + k_o^2\,(n^2(x) - s^2)V = \frac{d\ln(\mu-s^2/\varepsilon)}{dx}\frac{dV}{dx} \tag{4.2}$$

for TM waves and

$$\frac{d^2U}{dx^2} + k_o^2\,(n^2(x) - s^2)U = \frac{d\ln\mu}{dx}\frac{dU}{dx} \tag{4.3}$$

and

$$\frac{d^2V}{dx^2} + k_o^2\,(n^2(x) - s^2)V = \frac{d\ln(\varepsilon-s^2/\mu)}{dx}\frac{dV}{dx} \tag{4.4}$$

for TE waves. Even if μ is a constant, ε will not be. If ε varies slowly we may make a WBKB approximation[2,3] and set the right side of these equations equal to zero. In general, this approximation will not be valid. It can serve as a good starting point for perturbation theory, it makes contact with a large body of literature, and it is instructive. Therefore we will consider solutions to the equation

$$\frac{d^2\psi}{dx^2} + k_o^2(n^2(x) - s^2)\ \psi = 0 \quad . \tag{4.5}$$

Without loss of generality, we may simplify our discussion by setting $s^2 = 0$ (normal incidence).

In mechanics we have[4]

$$n(x) \sim \sqrt{(E - V(x))/E} \tag{4.6}$$

where E is the energy and V(x) is the potential. In the particular case of quantum mechanics, we have

$$k = p/h \quad ,$$

and an equation of the form Equation (4.5) which is Schroedinger's equation. A great deal of work has been done on periodic systems using this equation in the band theory of solids. n corresponds to the impedance z in transmission line problems. In acoustics, we have $n \sim \rho v$, for velocity v and density ρ.[5]

4.1 Piecewise Constant Modulation

The step function modulation is one of the most thoroughly analyzed of any periodic response function.[6-28] It is easy to construct experimentally, can be solved exactly, and has cosines and sines for eigenfunctions, so that products of eigenfunctions can often be reduced to a compact form. Since the system is piecewise solvable, we may multiply matrices of the form

$$\begin{bmatrix} \cos k_o n_i \ell_i & n_i^{-1} \sin k_o n_i \ell_i \\ -n_i \sin k_o n_i \ell_i & \cos k_o n_i \ell_i \end{bmatrix} \tag{4.7}$$

for each layer of thickness ℓ_i and index n_i. The most studied case is the double layer (one atom), with periods a and b and indices n_a and n_b. After multiplying matrices, we obtain the dispersion relation from Equation (3.1):

$$\cos kd = \cos k_o n_a a \cos k_o n_b b - \frac{1}{2}\left(\frac{n_a}{n_b} + \frac{n_b}{n_a}\right) \sin k_o n_a a \sin k_o n_b b \quad . \tag{4.8}$$

Here $d = a + b$. We see that when $n_a \to n_b = n$, we find

$$\cos kd = \cos k_o n(a + b) \quad , \tag{4.9}$$

as we should. When $n_a << n_b$ and $a \sim b$ we find

$$\cos kd \approx \cos k_o n_b b - \frac{1}{2} k_o n_b a \sin k_o n_b b \quad . \tag{4.10}$$

A problem of more widespread interest occurs when $n_b b << n_a a$, but $n_b >> n_a$. Then we have

$$\cos kd \approx \cos k_o n_a a - \frac{1}{2} (n_b/n_a) k_b b \sin k_o n_a a, \tag{4.11}$$

where $k_b = k_o n_b$. This system was studied by Mason in regard to acoustic filters as early as 1927,[9] but is best known as the Kronig-Penney problem, after these authors published their independent derivation of the solution applied to a model of energy bands in solids in 1931.[10] Usually a variable n_e is defined in such a way that

$$n_e a = \frac{1}{2}(n_b/n_a)k_b b \quad . \tag{4.12}$$

Using Equation (4.6), with $V(x) = -U >> E$ over region b, $V(x) = 0$ over region a, and $E = k_o^2$ we have $n_a = 1$ and $n_b^2 \approx U/E$, so that $\frac{1}{2} n_b^2 k_o b/n_a \to \frac{1}{2} Ub/k_o$. This is commonly written as U'a.[10] this model is commonly used for energy band calculations.[11-15] If we make the association $n_a \sim z_a$, $\frac{1}{2} k_o b n_b = n_b' = z_b$, we make contact with the problem of a transmission line with unloaded line impedance z_a that is loaded at distances a apart by discrete impedances z_b:

$$\cos kd \simeq \cos k_o n_a a - (z_b/z_a) \sin k_o n_a a \quad . \qquad (4.13)$$

For a string or rod loaded by point masses, $z_b = m\omega$.[5] If we now consider only long wavelength waves, we may write:

$$1 - \cos kd \simeq (n_b'/n_a)\, k_o n_a a \quad , \qquad (4.14)$$

or

$$2 \sin^2 (\tfrac{1}{2}\, kd) \simeq k_o n_b' a \quad , \qquad (4.15)$$

making contact with the literature on lattice dynamics.

The double periodic square well potential has been studied by Dubrovskii and Pogorelskii;[14] the resulting expression for the dispersion relation is complicated.

4.2 Sinusoidal Modulation

Another problem that can be solved exactly is that in which the potential is sinusoidal. This was first treated by Morse in 1930.[29] Morse solved the problem in three dimensions as well as in one dimension. We write $\varepsilon(x)$ as

$$\varepsilon(x) = \varepsilon_o - \varepsilon_1 \cos(2\pi x/a) \quad . \qquad (4.16)$$

and letting

$$\alpha = k_o^2 \varepsilon_o \quad , \quad q = \frac{1}{2} k_o^2 \varepsilon_1 \quad , \text{ and } \varepsilon = \varepsilon^2 \qquad (4.17)$$

we may write Equation (4.5) (with s = 0) as

$$d^2\psi \,/\, dx^2 = [\alpha - 2q\cos(2\pi x/a)]\psi \quad . \qquad (4.18)$$

This is the standard form of Mathieu's equation.[30] The solutions are circular elliptic functions. There are four basic types of these functions:

$$ce_{2n}(z,q) = \sum_r A_{2r} \cos 2rz \quad , \tag{4.19}$$

$$ce_{2n+1}(z,q) = \sum_r A_{2r+1} \cos(2r+1)z \quad , \tag{4.20}$$

$$se_{2n+1}(z,q) = \sum_r B_{2r+1} \sin(2r+1)z \quad , \tag{4.21}$$

and

$$se_{2n+2}(z,q) = \sum_r B_{2r+z} \sin(2r+2)z \quad , \tag{4.22}$$

where $z = \pi x/a$ and should not be confused with the impedence. The functions ce_m and se_m go over to cosine and sine functions when ε_1 is small compared to ε_o. Some of them are shown in Figure 4.1. The Mathieu functions may also be expanded in terms of cylindrical Bessel functions and Hankel functions, and in the case of large q, may be approximated by parabolic cylinder functions.[31] We will discuss various expansions of the Mathieu functions in Section 6.

Levine has examined the effect of various terminations on the stop and pass bands pertaining to the Mathieu problem. Perturbations were studied by Slater,[32] who considered a dielectric of the form $\varepsilon_o + \varepsilon_1 \cos 2z + \varepsilon_2 \cos 2pz$, as well as $\varepsilon_o + \varepsilon_1 \cos 2z + \varepsilon_2 \cos z$. Slater considered two- and three-dimensional perturbation problems as well as the one-dimensional problem.

4.3 General Observations

Since both the Kronig-Penney and the Mathieu problems are exactly solvable, comparisons have been made of the stop and pass bands created by these modulation profiles. The result depends on the relative size of the distances a and b in the Kronig-Penney profile. When a ≃ b, the two profiles give very

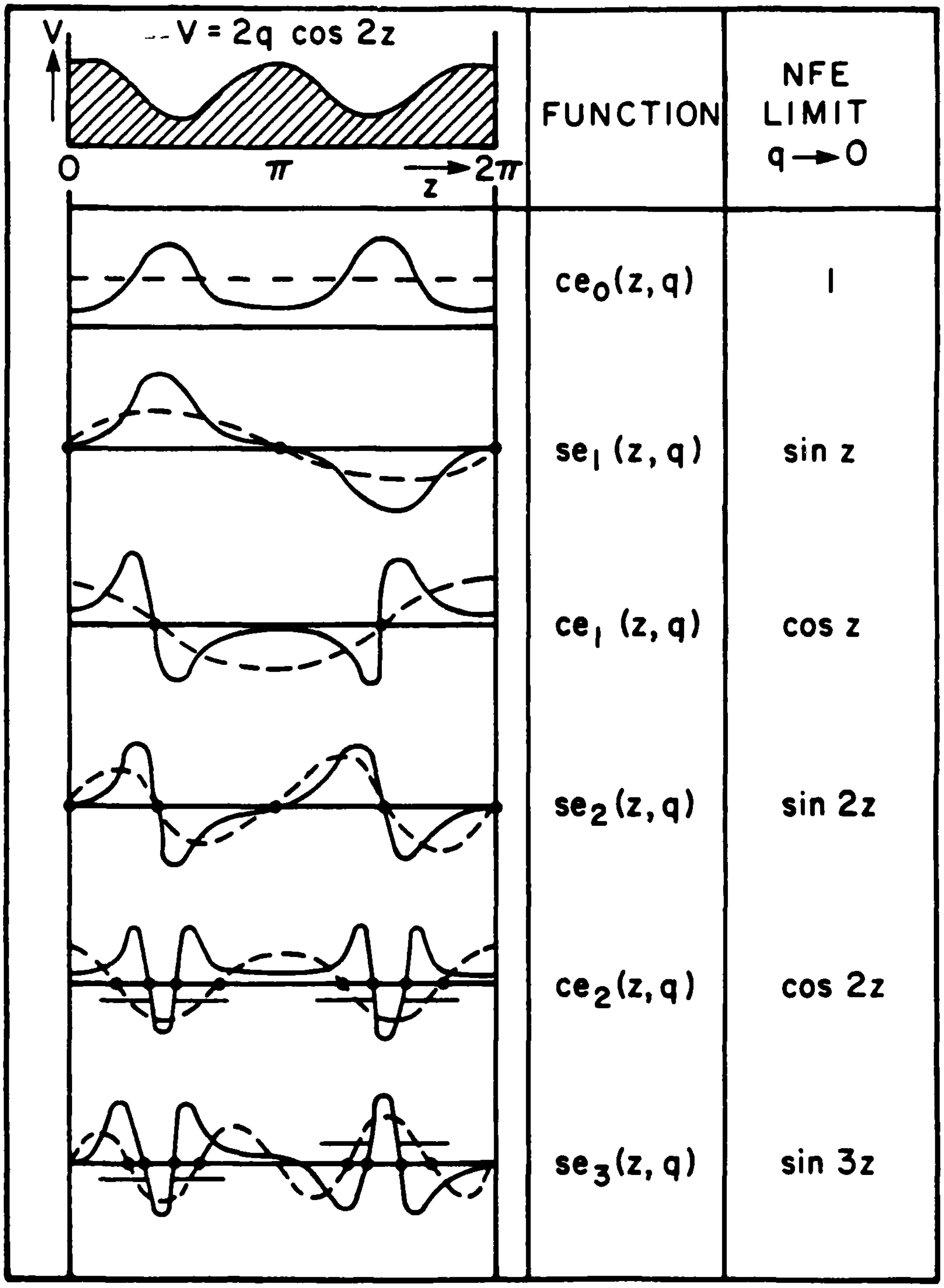
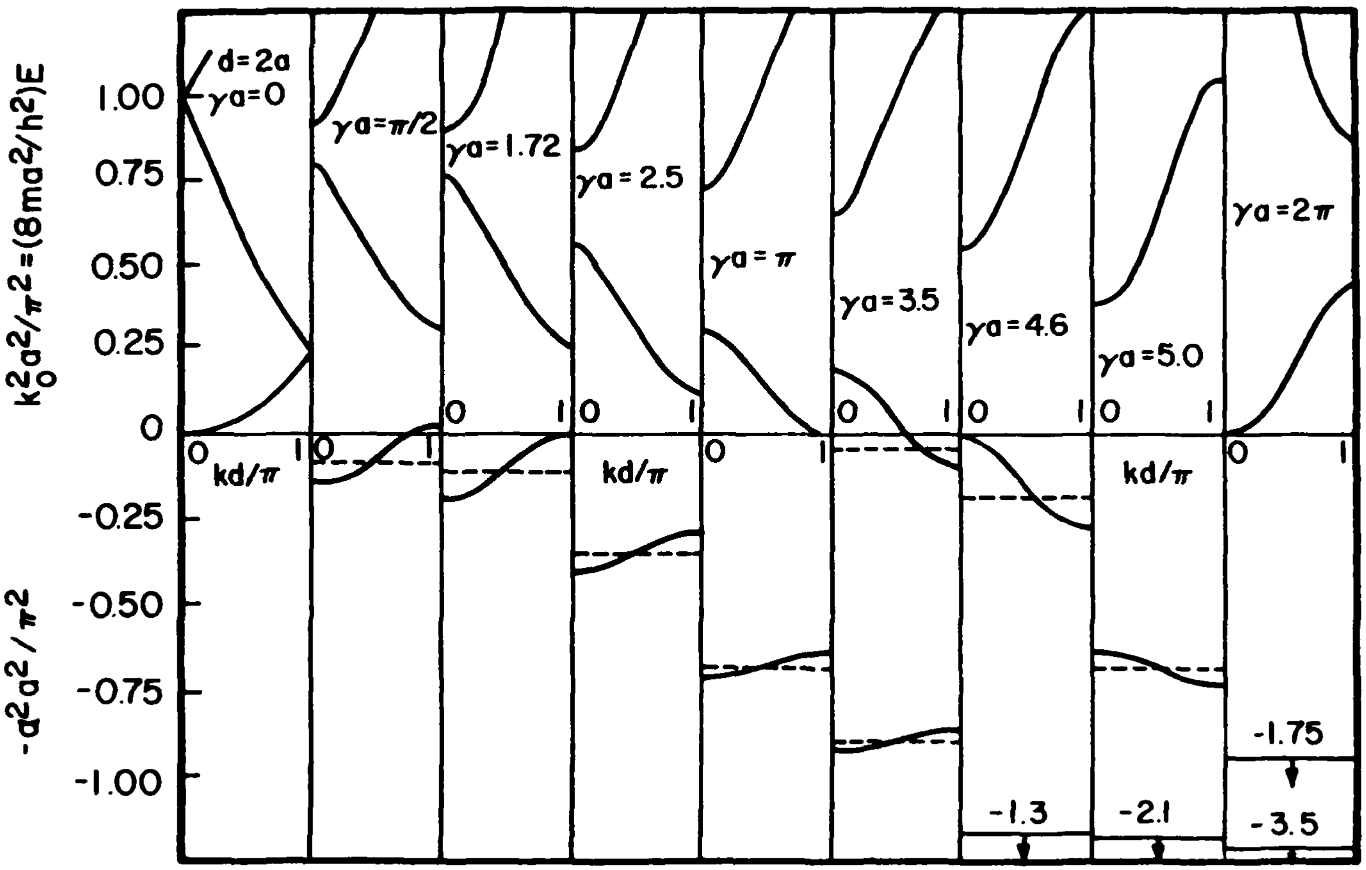


Figure 9. Form for Mathieu functions.

similar results. The width of the pass bands relative to the stop bands increases with the ratio of b/a.[33]

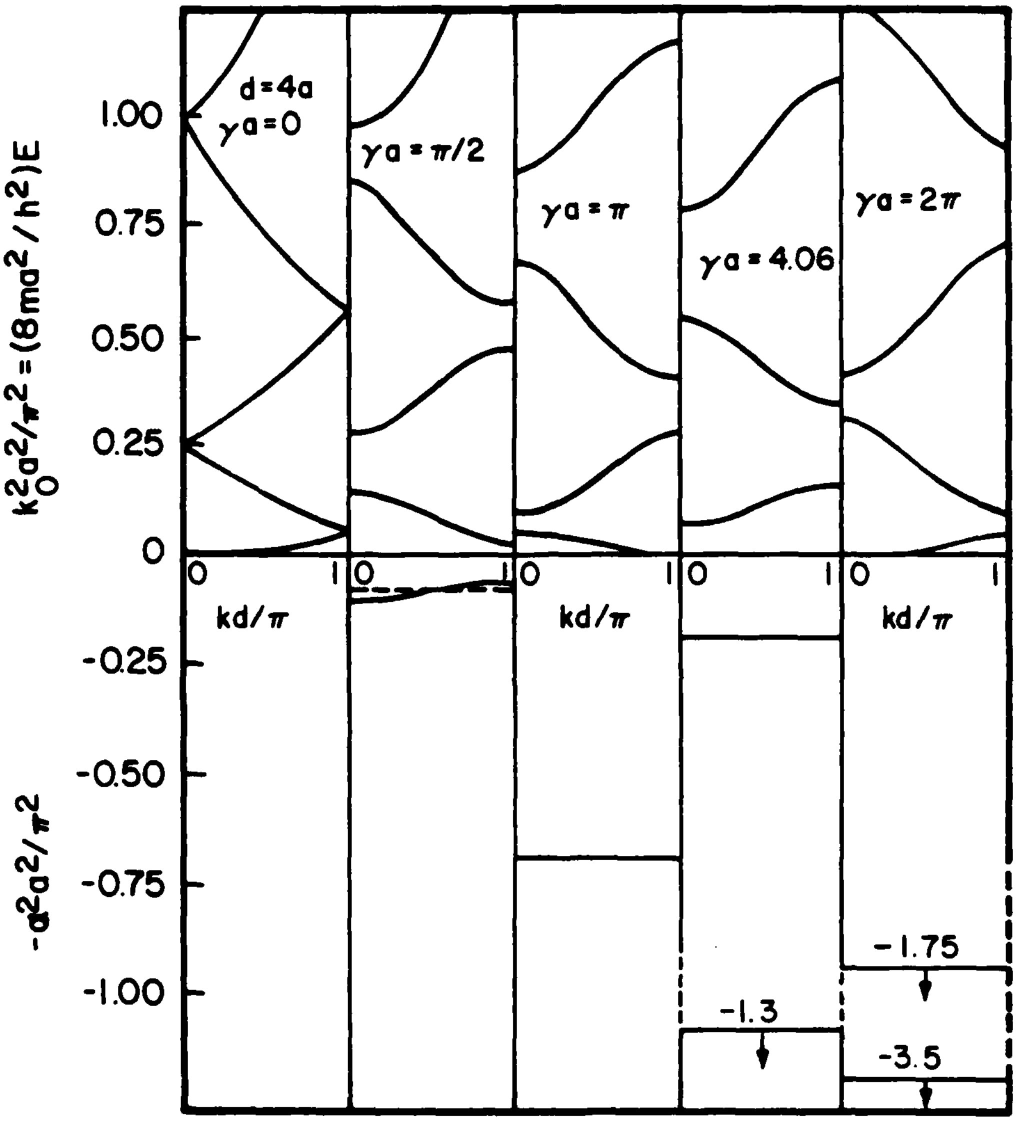
As a wave propagates through the filter, it is partly reflected due to modulations in the refractive index. If the wavelength is much greater that the periodicity in ($\bar{n}k_o d \ll 1$ for a mean index $\bar{n}$), the wave will not see the index modulation, and the wave will be passed. When the wavelength in the medium nearly matches d, the wave will interact strongly with the modulated profile; constructive interference will occur between reflections that occur at distances d apart. This will also occur at wavelengths which are submultiples of this critical wavelength--a series of stop and pass bands will occur. Examples corresponding to Equation (4.10) are given in Figures 4.2 and 4.3, where $\gamma \sim n_b - n_a$. The width of the stop bands is roughly proportional to the amplitude of the index modulation.

By our argument, we see that successive stop bands arise in part from the corresponding Fourier components of the modulation profile. Thus the second stop band is sensitive to the strength of the second Fourier component of the index modulation, etc. Consequently the widths and positions of the lowest bands are not very sensitive to changes in the modulation profile, only to its periodicity (length of the unit cell). Changes in the shape of the profile have their greatest effect on the higher-order bands. For example, if we approximate a sinusoidal index modulation by a series of thin steps, we may expect very little effect on the location of the edges of the lowest bands. At high bands corresponding to wavelengths on the order of the step thickness, we would anticipate relatively large changes. Of course, these higher order bands may well correspond to wavelengths that lie above the bandgap of the dielectric materials. If the step thickness is 100 nm, then we would expect strong changes in the bands corresponding to energies of say 10eV. However, this



Energy bands for various values of γa, with $d = 2a$

Figure 10. Dispersion curves for square well problem as a function of modulation depth, for d = 2a.



Energy bands for various values of γa, with $d = 4a$

Figure 11. Dispersion curves for d = 4a.

region is not of particular interest. In other words, the modulation depth and overall periodicity d are the main parameters affecting the band edges of interest. Fine details of the shape of the modulation are not very important. Bands corresponding to the Mathieu problem are shown in Figures 4.4 and 4.5. A comparison between the bands for the Kronig Penney and Mathieu problems is shown in Figures 4.6 and 4.7.

If the system is multiple, periodic higher-order bands at corresponding multiples will be affected. We will discuss this further in the next section, but we can see from the argument given above that since a multiple periodicity implies that second and higher order Fourier components of the modulation profile will be large, the stop bands (band gaps) above the fundamental will be widened.

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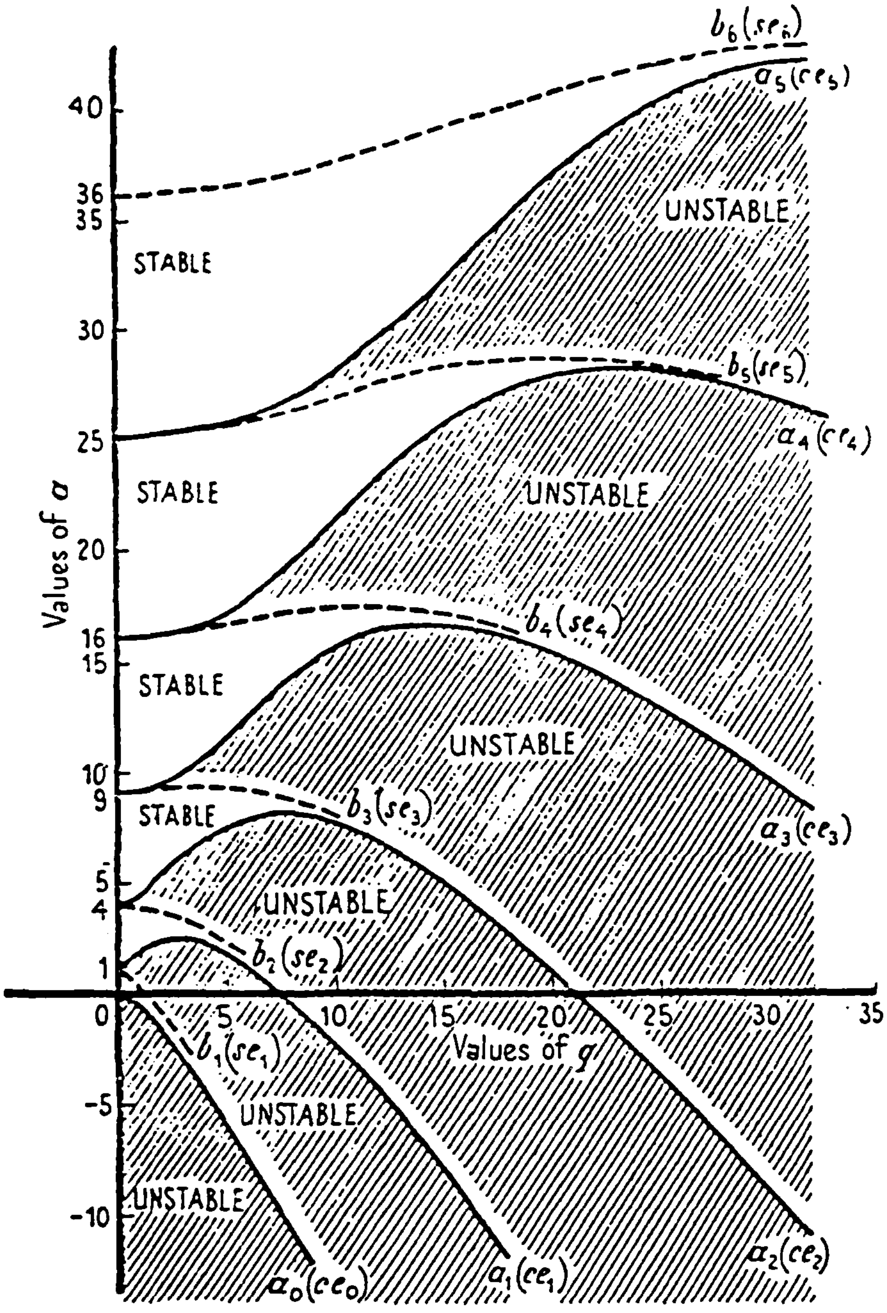

STABILITY CHART FOR MATHIEU FUNCTIONS

INTEGRAL ORDER

Figure 12. Allowed regions of solutions for the Mathieu problem as function of q.

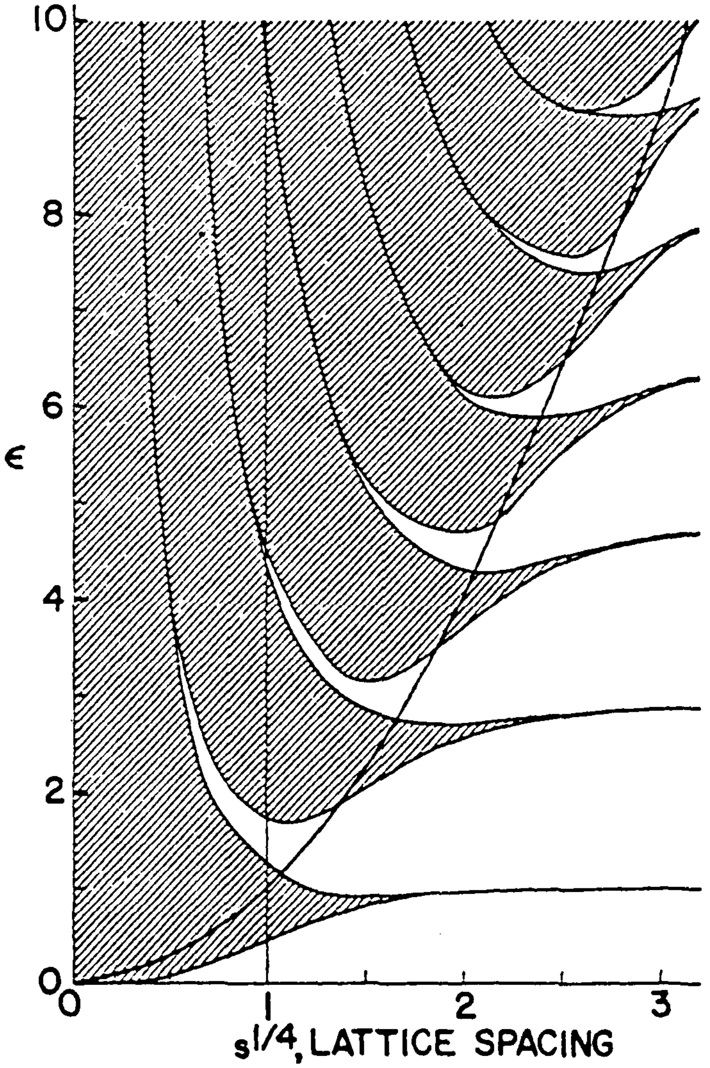

Figure 13. Allowed regions of solution for the Mathieu problem.

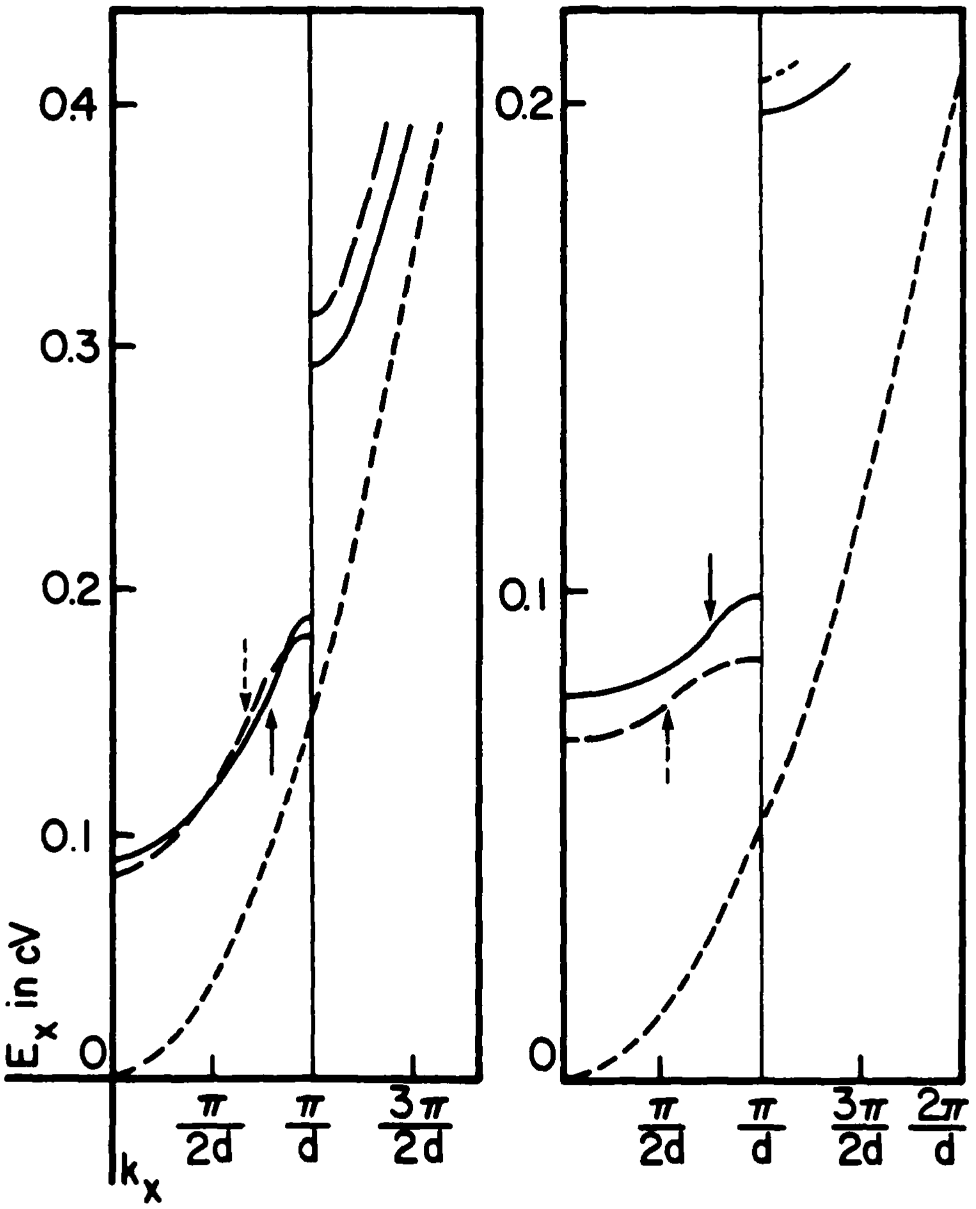

Figure 14. Comparison between square-well and Mathieu dispersion curves.

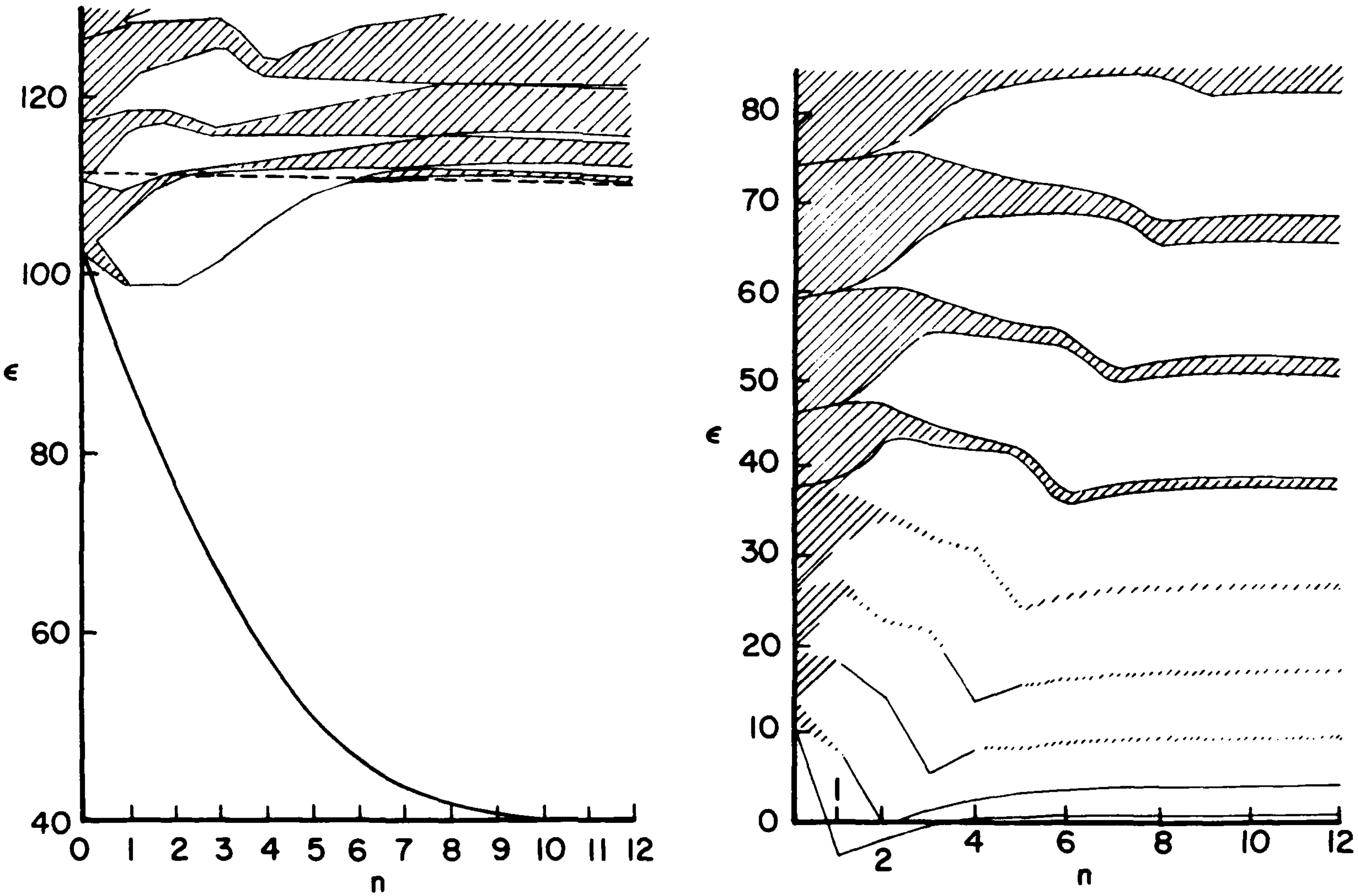

Figure 15. Behaviour of stop and pass bands as a function of the a/b ratio.

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5. DIFFERENCE EQUATION CALCULATIONS

Often we can convert a PDE into a difference equation by an appropriate series transformation or decomposition, followed by an approximation which allows us to limit the coupling that occurs between the basis states of the decomposition. We now give two examples of how this can be done. The first is a Fourier transformation; the second is known as the tight binding, or LCAO method. It is the approximation which limits the number of connected basis states appearing in the difference equation that makes the difference equation method practical. consequently, this approach is only useful when such an approximation can be made.

5.1 Fourier Transformation[1,2]

We wish to solve the PDE of the form in Equation (4.5). We make the decompositions

$$\psi_k(x) = \sum_j A_j(k)\, e^{ik_j x} , \tag{5.1}$$

where

$$k_j = k + 2\pi j/d , \tag{5.2}$$

and

$$n^2(x) = \sum_\ell g_\ell e^{iK_\ell x} , \tag{5.3}$$

where

$$K_\ell = 2\pi\ell/d .$$

Substituting Equations (5.2) and (5.3) in (4.5), we find

$$\sum_j [(k + k_j)^2 + k_o^2[s^2 - \sum_\ell g_\ell e^{iK_\ell x})] A_j(k) e^{ik_j x} = 0 \quad . \quad (5.4)$$

In principle, Equation (5.4) is exact, but involves an infinite sum over the Fourier components g_ℓ for the square of the index, n^2. We need to drastically reduce the number of these components. Fortunately, if $n^2(x)$ is a reasonably smooth function, we may terminate the series in ℓ after a few terms. As an example, we consider the Mathieu problem, in which we have

$$g_\ell = g\delta_{\ell\pm 1} \quad . \quad (5.5)$$

Substitution of Equation (5.5) into Equation (5.4) now gives

$$[(k + k_j)^2 + k_o^2 s^2] A_j = k_0^2 [A_{j-1} + A_{j+1}] \quad . \quad (5.6)$$

This is a solvable equation. Rather than pursue it here, we go on to derive a similar equation by another means.

5.2 Tight-Binding Approximation[3]

A great deal of work has been done using difference equation calculations in the band theory of solids based on the tight-binding approximation.[3-12] This corresponds to the case in which regions of large refractive index are sufficiently separated by regions of low refractive index that they form optical wells which are only weakly coupled. Parallel calculations have been made in three dimensions as well as one dimension and include investigation of the effect of various terminations (surface states). Although they are most accurate in cases of very deep modulation of the index profile, they provide an instructive insight into band behavior, and serve as good points for comparison with more general calulations.

Let us assume that we have a complete set of known orthonormal solutions ϕ_n for the equation

$$\phi_n'' + k_o^2[n_o^2(x) - s_o^2]\,\psi_n = 0 \quad , \tag{5.7}$$

and that we wish to solve Equation (4.5):

$$\psi'' + k_o^2[n^2(x) - s^2]\psi = 0 \quad , \tag{5.8}$$

for some

$$n^2(x) = n_o^2(x) + \eta^2(x) \quad . \tag{5.9}$$

We may expand ψ in terms of some as yet unknown coefficients a_n as follows:

$$\psi = \sum_n a_n \phi_n \quad . \tag{5.10}$$

Upon substitution of Equation (5.10) into Equation (5.8) we obtain

$$\sum_n a_n k_o^2[s^2 - s_o^2]\phi_n = \sum_n a_n k_o^2 \eta^2 \phi_n \quad . \tag{5.11}$$

If we multiply this equation of ϕ_m and integrate, we will obtain the results

$$\sum_n a_n k_o^2[s^2 - s_o^2] = \sum_n a_n k_o^2 \int dx\ \phi_m(x)\phi_n(x)\eta^2(x) \quad . \tag{5.12}$$

Since the functions $\phi_n(x)$ are known, the integrals are obtainable in principle, and we may solve for the coefficients a_n in terms of them. The result will be a series of coupled equations. This can get very messy if a given initial solution ϕ_m is coupled by $\eta(x)$ to very many other solutions ϕ_n. The conversion to a difference equation is only practical if the coupling is only to a few other solutions. An example in which this can occur is when the ϕ_n are localized in a region smaller than the (unit cell) distance d. We consider the case in which we have

$$\begin{aligned} \int dx\ \phi_m(x)\phi_n(x)\eta^2(x) &= \alpha \quad , \quad m = n \\ &= \beta \quad , \quad m = n \pm 1 \quad , \end{aligned}$$

$$= 0 \quad , \quad (m - n) > 1 \quad . \tag{5.13}$$

Then we will find

$$\beta(a_{n+1} + a_{n-1}) = (\bar{s} - \alpha)a_n \quad , \tag{5.14}$$

with $s^2 - s_o^2 = \bar{s}$. We see that we have greatly simplified the solution by our approximation. It has been found useful to assume that a_n is of the form

$$a_n = \lambda^n \tag{5.15}$$

Substitution of Equation (5.15) into Equation (5.14) yields

$$\lambda^{n-1} \left[\beta\lambda^2 - (\bar{s} - \alpha)\lambda + \beta\right] = 0 \quad . \tag{5.16}$$

We now rewrite Equation (5.16) as

$$\lambda^2 - \left[\frac{s-\alpha}{\beta}\right]\lambda + 1 = 0 \quad . \tag{5.17}$$

We note that Equation (5.17) is of the same form as the eigenvalue equation for the transfer matrix, B. That is, if we wish to solve the equation

$$\psi(x+d) = \lambda\psi(x) \quad , \tag{5.18}$$

we need to find the roots of the transfer matrix as given for example in Equation (3.28):

$$\begin{vmatrix} G(d) - \lambda & H(d) \\ G'(d) & H'(d) - \lambda \end{vmatrix} = 0 \quad . \tag{5.19}$$

This gives

$$\lambda^2 - \left[G(d) + H'(d)\right]\lambda + 1 = 0 \quad , \tag{5.20}$$

since det[B] = 1.

We know that the dispersion relation is

$$\mathrm{Tr}[B] = G + H' = 2\cos kd \quad , \tag{5.21}$$

and take advantage of this insight to make the assumption

$$(\bar{s} - \alpha)/\beta = 2\cos kd \quad . \tag{5.22}$$

Now if we substitute Equation (5.22) into Equation (5.17), we will find

$$\lambda = \cos kd \pm i\sin kd = e^{\pm ikd} \quad . \tag{5.23}$$

In turn, substitution of Equation (5.23) into Equation (5.15) will bring

$$a_n = Pe^{iknd} + Qe^{-iknd} \quad . \tag{5.24}$$

Since the basis functions ϕ_n were assumed to be known, the problem has now been solved given the appropriate boundary conditions. We see from Equation (5.24) that we have shown that the assumption Equation (5.22) implies that the expansion Equation (5.10) is in terms of Block waves. Usually the equivalence is derived in the other direction: the Block expansion allowed due to the periodicity of the system implies the condition Equation (5.21).[13,14] We note that Equations (5.6) and (5.14) are of similar form. This is in part due to our use of a Block expansion.

5.3 Surface States

We can investigate effects such as terminating the filter through the boundary conditions. We let the filter consist of N periods of length d, so that the filter has a length

$$L = Nd \quad . \tag{5.25}$$

We then impose the boundary condition that ψ be zero at L:

$$a_n = 0 \quad . \tag{5.26}$$

Together with Equation (5.24), Equation (5.26) implies that

$$a_n = A\sin(N - n)kd \,/\, \sin Nkd \quad . \tag{5.27}$$

Since A / sinNkd is simply a constant normalizing factor, we drop it in favor of

$$a_n = \sin(N - n)kd \quad . \tag{5.28}$$

We obtain our other boundary condition at the termination by making the substitution

$$\beta a_1 = (\bar{s} - \alpha')a_o \tag{5.29}$$

for Equation (5.14). Then Equations (5.28) and (5.29) give

$$(\bar{s} - \alpha')\sin Nkd = \beta\sin(n - 1)kd \quad . \tag{5.30}$$

From Equations (5.30) and (5.22) we get

$$(\alpha - \alpha')/\beta + 2\cos kd = \cos kd - \cot Nkd \sin kd \quad , \tag{5.31}$$

or, with

$$\zeta = (\alpha - \alpha') \,/\, \beta \quad , \tag{5.32}$$

$$\zeta = -\sin(N + 1)kd \,/\, \sin Nkd \quad . \tag{5.33}$$

The intersection of this family of curves with the curves $\zeta(kd)$ = constant yield solutions for $\zeta > 1$. One solution, corresponding to a_o, the "surface state," will give a complex value of k. This wave will not propagate through the filter.

The edges of the pass band are given by the dispersion relation Equation (5.22). The density of states will be greatest at the band edges.

5.4 Extensions and Multiple Periodicity

The difference equation tack is a useful means of studying the effects of multiple periodicity. The conversion to a difference equation has been used extensively for this purpose in band theory and lattice dynamics. The published literature is a valuable guide for parallel calculations which we might wish to make. However, the results that have been obtained in these fields are not readily used in optics, since energy band results seek to solve for the eigenvalues (or energy) of the Schroedinger equation, which is equivalent to solving for s in Equation (5.12) or $\bar{s}$ in Equation (5.14). We can easily take $\bar{s} = 0$, and wish to find the relation between k_o and k. We are also interested in an algorithm that is generally useful beyond the nearly free and tight binding approximations. It seems that this can be done. Let

$$\begin{bmatrix} \psi(x) \\ \\ \psi'(x) \end{bmatrix} = \vec{\psi}(x) \quad . \qquad (5.34)$$

Then

$$\vec{\psi}(x+d) = B(d)\vec{\psi}(x) \qquad (5.35)$$

and

$$\vec{\psi}(x-d) = B^{-1}(d)\vec{\psi}(x) \quad . \qquad (5.36)$$

Hence

$$\psi(x+d) + \psi(x-d) = \left[B(d) + B^{-1}(d)\right]\vec{\psi}(x) \quad . \qquad (5.37)$$

With

$$\psi(x+d) = e^{kd}\psi(x) \qquad (5.38)$$

and

$$\psi(x-d) = e^{-kd}\psi(x) \quad , \qquad (5.39)$$

we find

$$B(d) + B^{-1}(d) = 2\cosh(kd) \quad . \qquad (5.40)$$

From Equation (3.29) (and the discussion following it in Section 3) we have

$$B = \begin{bmatrix} G & H' \\ G' & H' \end{bmatrix} \quad . \qquad (5.41)$$

The inverse of B is

$$B^{-1} = \begin{bmatrix} H' & -H \\ -G' & G \end{bmatrix} \quad . \qquad (5.42)$$

Therefore we may write Equation (5.40) as

$$\begin{bmatrix} G+H' & 0 \\ 0 & G+H' \end{bmatrix} = 2\cosh(kd) \quad , \qquad (5.43)$$

or

$$(G+H') \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 2\cosh(kd) \quad . \qquad (5.44)$$

It seems that the difference method may be applied to a general problem, if the boundary conditions are suitably chosen with respect to the unit cell. This would be very useful for the analysis of a multiply periodic medium. Consider the system

$$\vec{\psi}_b = \beta\vec{\chi} \tag{5.45}$$

$$\vec{\psi}_{\bar{a}} = \alpha^{-1}\vec{\chi} \quad , \tag{5.46}$$

where the subscripts refer to distances with respect to the argument of the r.h.s. We find

$$\vec{\psi}_b + \vec{\psi}_a = (\beta + \alpha^{-1})\vec{\chi} \quad . \tag{5.47}$$

Now

$$\vec{\chi}_a = \alpha\,\vec{\psi} \tag{5.48}$$

and

$$\vec{\chi}_{\bar{b}} = \beta^{-1}\vec{\psi} \quad . \tag{5.49}$$

Therefore

$$\vec{\chi}_a + \vec{\chi}_{\bar{b}} = (\alpha + \beta^{-1})\vec{\psi} \quad . \tag{5.50}$$

From Equations (5.47) and (5.50) we get

$$\begin{aligned} (\beta + \alpha^{-1})\,(\alpha + \beta^{-1})\vec{\psi} &= (\beta + \alpha^{-1})\,(\vec{\chi}_a + \vec{\chi}_{\bar{b}}) \\ &= \vec{\psi}_{b+a} + \vec{\psi} + \vec{\psi} + \vec{\psi}_{\bar{a}+\bar{b}} \\ &= \vec{\psi}_d + 2\vec{\psi} + \vec{\psi}_{\bar{d}} \quad . \end{aligned} \tag{5.51}$$

We write Equation (5.51) as

$$[(\beta + \alpha^{-1})(\alpha + \beta^{-1}) - 2]\psi = \psi_d + \psi_{\bar{d}} \quad . \tag{5.52}$$

With

$$\psi_d = \lambda\psi \tag{5.53}$$

and

$$\psi_{\bar{d}} = \lambda^{-1}\psi \tag{5.54}$$

we have

$$(\beta + \alpha^{-1})(\alpha + \beta^{-1}) - 2 = \lambda + \lambda^{-1} \quad , \tag{5.55}$$

or

$$\beta\alpha + \alpha^{-1}\beta^{-1} = \lambda + \lambda^{-1} \quad . \tag{5.56}$$

We let

$$M = \beta\alpha \tag{5.57}$$

and

$$\lambda = e^{kd} \quad . \tag{5.58}$$

Then we have

$$Tr[M] = \cosh kd \quad . \tag{5.59}$$

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6. PERTURBATION EXPANSIONS

We now look at some of the ways in which we can find approximate solutions for ψ and for the dispersion relation when the index modulation has a small departure about a profile for which we can solve.

6.1 Pedestrian Expansion

If we know that our modulation profile is similar to one for which we have a closed form solution we may make expansions about both the known solution and its corresponding modulation profile.[1] We let the known solution be ψ_1, and the unknown solution be ψ. We then write

$$\psi \approx \psi_1 + \delta_1 \psi_2 + \delta_1^2 \psi_3 \quad , \delta_1 << 1 \quad . \tag{6.1}$$

As δ_1 increases, we will need to include more terms in the expansion for ψ. Similarly, if the dielectric constant for the known case goes like $n_1^2(xl)$, we write

$$n^2(x) = n_1^2(x) + \delta_2 n_2^2(x) + \delta_2^2 n_3^2(x) \tag{6.2}$$

for $n_2(x)$ in the unknown case. Then, upon substituting Equations (6.1) and (6.2) into Equation (4.5) with $s^2 = 0$:

$$d^2\psi/dx^2 + k^2 n^2(x)\psi = 0 \quad , \tag{6.3}$$

we obtain

$$d^2(\psi_1 + \delta_1\psi_2 + \delta_1^2\psi_3)/dx^2 +$$

$$k^2(n_1^2 + \delta_2 n_2^2 + \delta_2^2 n_3^2)(\psi_1 + \delta_1\psi_2 + \delta_2^2\psi_3) = 0 \quad . \tag{6.4}$$

We can separate terms of a given order and arrive at a series of equations:

$$\psi_1'' + k^2 n_1^2 \psi_1 = 0 \quad , \tag{6.5}$$

$$\psi_2'' + k^2 n_1^2 \psi_2 = -(\delta_2/\delta_1) n_2^2 \psi_1 \quad , \tag{6.6}$$

and

$$\psi_3'' + k^2 n_1^2 \psi_3 = -(\delta_2/\delta_1) n_2^2 \psi_2 - (\delta_2/\delta_1)^2 n_3^2 \psi_1 \quad . \tag{6.7}$$

Equation (6.5) is our solvable homogeneous equation with a known solution. Equations (6.6) and (6.7) are similar to Equation (6.5) but are inhomogeneous. We can think of Equation (6.6) as a problem in which the solution to Equation (6.5) drives an oscillator of the same form as that of Equation (6.5).

We can learn something about the dispersion relation (k_o versus k) if the amplitude of the index modulation is small by making another expansion, similar to that of Equation (5.1). We write

$$\psi_k(x) = \sum_j A_j(k) e^{ik_j x} \quad , \tag{6.8}$$

with

$$k_j = k + 2\pi j/d \quad . \tag{6.9}$$

6.2 Band Gap for Small Perturbations

We assume a small perturbation in the index modulation about a value for which we can solve. Then we have[2,3]

$$\psi_k(x) = A_m e^{ik_m x} + \delta_1 {\sum_j}' A_j e^{ik_j x} \quad . \tag{6.10}$$

We begin by letting m = 0. We write our equation for ψ as

$$\psi'' + k_o^2 (n_0^2 + \delta_2 n_1^2) \psi = 0, \tag{6.11}$$

with

$$n_1^2 = \sum_\ell g_\ell e^{iK_\ell x} \quad , \tag{6.12}$$

and

$$K_\ell = 2\pi \ell / d \quad . \tag{6.13}$$

Then we substitute Equations (6.9), (6.10), and (6.12) into Equation (6.11) and find

$$\begin{aligned} A_o (k_o^2 n_o^2 - k^2) e^{ikx} &+ \delta_1 {\sum_j}' (k_o^2 n_o^2 - k_j^2) A_j e^{ik_j x} \\ &+ \delta_2 k_o^2 A_o \sum_\ell g_\ell e^{iK_\ell x} \\ &+ \delta_1 \delta_2 k_o^2 {\sum_j}' \sum_\ell g_\ell A_j e^{i(k_j + K_\ell) x} = 0. \end{aligned} \tag{6.14}$$

To first order we let

$$\delta_1 = \delta_2 = \delta \quad .$$

Then to first order we have approximately[2]

$$\begin{aligned} &A_o (k_o^2 n_o^2 - k^2) e^{ikx} \\ &\quad + \delta {\sum_j}' [(k_o^2 n_o^2 - k_j^2) A_j + A_o k_o^2 g_\ell] e^{ik_j x} \approx 0 \quad . \end{aligned} \tag{6.15}$$

We now operate on Equation (6.15) with

$$\int_0^d dx\, e^{-ik_jx} \quad .$$

We find

$$k = n_o k_o \quad , \quad j = 0 \quad . \tag{6.16}$$

$$A_j = \frac{k_o^{\,2}}{k_j^2 - n_o^2 k_o^2}\, g_\ell A_o \quad , \quad j \neq 0 \quad . \tag{6.17}$$

We see that to first order in δ, k is unchanged, and the form for ψ is modified slightly. If we operate with

$$\int_0^d dx e^{-ikx}$$

we find to second order in δ (see Reference 2)

$$A_o(k_o^2 n_o^2 - k^2)d + \delta_1 \delta_2 \sum_j{}' \sum_\ell A_j g_\ell \int_0^d dx e^{i(k_j + K_\ell - k)x} = 0 \quad . \tag{6.18}$$

The integral vanishes, unless

$$\ell = -j \quad . \tag{6.19}$$

Hence

$$A_o(k_o^2 n_o^2 - k^2) + \delta_1 \delta_2 \sum_j{}' A_j g_{-j} = 0 \quad . \tag{6.20}$$

From Equation (6.17), we find

$$k^2 = k_o^2 n_o^2 + \delta_1 \delta_2 \sum_j{}' \frac{k_o^{\,2}}{k_j^2 - n_o^2 k^2}\, g_j g_{-j} \quad . \tag{6.21}$$

We see that a problem develops in Equations (6.17) and (6.21) when $k \to k_j$. We can patch this up by increasing the contribution from the mth term:

$$\psi = A_o e^{ikx} + A_m e^{ik_m x} + \delta_1 \sum_j{}'' A_j e^{ik_j x} \quad . \tag{6.22}$$

Then proceeding as before, we find to first order

$$A_o(n_o^2 k_o^2 - k^2) + \delta k_o^2 A_m g_m = 0 \tag{6.23}$$

and

$$\delta k_o^2 A_o g_{-m} + (n_o^2 k_o^2 - k_{-m}^2) A_m = 0 \quad . \tag{6.24}$$

Hence

$$(n_o^2 k_o^2 - k^2)\,(n_o^2 k_o^2 - k_{-m}^2) = \delta^2 k_o^2 \mid g_m \mid^2 \; . \tag{6.25}$$

For $k \approx k_{-m}$ we find approximately

$$k_o^2 \approx k_{\overset{-}{m}}^2 \,/\, (n_o^2 + \delta g_m) \quad . \tag{6.26}$$

This creates a band gap with width

$$\Delta k = \frac{g_m}{2n_o^2}\, k_m = \frac{g_m}{2\varepsilon_o}\, k_m \quad . \tag{6.27}$$

This means that a stop band is formed whose width for the mth band is proportional to the mth component of n_1^2.

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7. CANDIDATE MATERIALS

The impetus for this report was a literature survey of suitable candidate materials for graded index optical components and devices. Such an undertaking would be a prodigious task, especially in view of the limited data available on the optical properties of materials, and the vast number of possibilities. This is all the more true because of the decision to direct the bulk of the effort of this work to the analysis discussed in the first six sections of this report. Nevertheless, the author wishes to present his initial impressions of the possibilities for suitable materials, albeit from the prospective of a novice and an outsider, and to report on a limited literature survey. First, some general considerations and comments are in order.

7.1 General Comments

The throughput of an optical device and its immunity to damage under high-power conditions will be enhanced if the absorption is low for a given optical path length, i.e., if $n_i << n_r$. This mitigates against the use of amorphous materials, which in practice tend to suffer from large absorption. This is due in part to a very high density of scattering centers arising from local, microscopic inhomogeneities, such as the frequent occurrence of voids, and a general tendency to a high density of impurities. This is especially likely if the stoichiometry must be varied over a wide range. The latter problem is no doubt enhanced by the former difficulties. Furthermore, amorphous materials tend to possess wide regions over which infrared radiation is absorbed by photons. Since we wish to vary the refractive index continuously, a second implication of the need to minimize absorption and scattering is the high desirability of using materials with good mutual solubility; we seek compounds possessing a similar structure with as different a refractive index as possible. The third corollary is the requirement that the chosen compounds be amenable to manufacture with a low concentration of defects.

The chosen materials should be rugged, that is, they should be chemically resistant, especially to moisture, should have good mechanical strength, and a high phase transition temperature. Their refractive index should not vary rapidly with temperature. The desirability of minimizing short-range disorder suggests that the solid solute materials be chosen with nearly equal bond lengths as well as identical structures. This will be especially true if the creation of a single crystal device is attempted. A basic premise of the following presentation is that the bonding lengths will usually be dominated by the nonmetals in the compounds, rather than the metals.

This can be seen from Table 1, which gives the radii of several atoms of interest.[1] We note that covalent bond lengths are especially likely to be dominated by the identity of the nonmetal atoms. In these cases the small metal atoms often fit into voids created by nearly close-packed nonmetal atoms. Thus we may expect to vary physical properties without significantly affecting bond lengths by substituting different metal atoms with a given nonmetal atom. A good example of this occurs for compounds of transition metal atoms with chalcogenide atoms. Assuming that this hypothesis is true, we should seek compounds with identical structures, different cations, and anions which are either identical or of nearly the same size.

To ensure structural compatibility in a solution, we will also restrict ourselves to groups of atoms which form compounds with the same structure as well as closely matched lattice parameters when all possible combinations of atoms are considered. Therefore, we will organize our discussion in terms of crystal structure in general, and in terms of the chemical

TABLE 1

CRYSTAL RADII

Li	Be	B	C	N	O	F
0.60	0.31	0.20	2.60	1.71	1.40	1.36
Ns	Mh	Al	Si	P	S	Cl
0.95	0.65	0.50	2.71	2.12	1.84	1.81
Cu	Zn	Ga	Ge	As	Se	Br
0.96	0.74	0.62	2.72	2.22	1.98	1.95
K	Ca	Se	Ti	V	Co	
1.33	0.99	0.81	0.68	0.59	0.52	
Rb	Sr	Y	Zr	Nb	Mo	
1.45	1.13	0.93	0.80	0.70	0.62	
Ag	Cd	In	Sn	Sb	Te	I
1.26	0.97	0.81	2.94	2.45	2.21	2.16
Cs	Ba	La	H_f	Ta	W	
1.69	1.35	1.15	0.78	0.68	0.70	
	Hg	Tl	Pb			
	1.10	0.95	0.84			

properties of the anions in particular. Since we did not consider dispersion in the earlier sections we will not give it much attention below. Also, we will concentrate on linear refractive indices. Finally, we will concentrate on simple compounds, as they should have fewer absorption bands in the infrared.

The optical behavior of a compound is strongly affected by the chemical nature of its bonds, in an analogous manner to many of its other properties. It appears to the author that the ionic materials often have the desirable attributes of low optical absorption, low defect concentrations, and high melting points, as well as wide band gaps. In many instances, especially in the case of the halogens, they are subject to chemical attack, particularly by water, and often they are brittle. However, a more serious difficulty is that ionic compounds tend to have low indices of refraction, and a range of refractive indices extending to high values is often desirable.

7.2 Halides

The fluoride compounds form a group of highly ionic materials that have well developed and well understood optical properties. They have very low absorption coefficients. However, their refractive indices are uniformly low (n_r ranges from 1.25 to 1.53) seriously restricting their versatility. Some of the pertinent properties of several fluoride compounds are given in Table 2. In the tables, a is the lattice constant (all lattice constants in the tables are given in angstroms), ε_∞ is the high-frequency dielectric constant, ε_s is the static dielectric constant, and ω_t and ω_L are respectively the transverse and longitudinal optical photon frequencies at the gamma point in cm^{-1}. Gisin[2] found that films of SrF_2 showed improved performance with increasing substrate temperature during

TABLE 2

FLUORITE STRUCTURE

Compound	a	n(μm)			ε_s
		.5	2	5	
CdF_2	5.388	1.		1.53	
CaF_2	5.463	1.437	1.43-1.46	1.424	6.8
HgF_2	5.54				
EuF_2	5.796				
SrF_2	5.800		1.25-1.36		7.69
PbF_2	5.927				
BaF_2	6.200	1.478	1.38-1.53	1.451	7.33
$SrCl_2$	6.977				9.19
$BaCl_2$	7.34				
YL_iF_4			1.458		

formation. This was attributed to a decrease in porosity. Gisin states that the optical constants of films of SrF_2 depend on the layer thickness due to nonuniform stoichiometry. Hall[3] found that the index, absortion, and crystallinity of MgF_2 increased with age. Hall attributes the increased absorption to the creation of vacancies with the onset of crystallization. Barnes and Gettemy[4] reported on the optical properties of $LiYF_4$, which has a very low temperature coefficient.

The CsCl materials also have low dielectric constants. Data on these compounds are given in Table 3, much of which is taken from Brown,[5] Burstein et al.,[6] Lucovsky, et al.,[7] and to a lesser extent, Rao.[8] (These authors are also the main basis for Tables 4, 15, and 24.) The best bet for this group of materials appears to be either $TlCl/NH_4Cl$ or TlCl/TlBr. There is a wider selection of NaCl structure materials with a fairly wide range of dielectric constants (see Table 4). Unfortunately, the alkalai halides can develop color centers.[5] This may present a problem for work in the visible, but the $Ag_xNa_{1-x}Br$ and $Ag_xNa_{1-x}Cl$ systems appear to be attractive for work in the infrared. In most ionic compounds, we expect only a 10% change in the dielectric constant for two materials with closely matched lattice parameters, but in these cases we find a change of almost a factor of 2.

Compounds of the halides with many of the transition metals have a layered structure. In these materials the small cations are trigonally coordinated with the larger anions (see Figure 7.1a). There are also layered compounds of chalcogenide atoms, which we will discuss below. In these materials the basic structure consists of three parallel planes. The two outer planes are made up entirely of anions. The middle plane consists only of cations. A sandwich structure results, with the sheet of metal atoms inside the sandwich, and all chemical bonds directed into

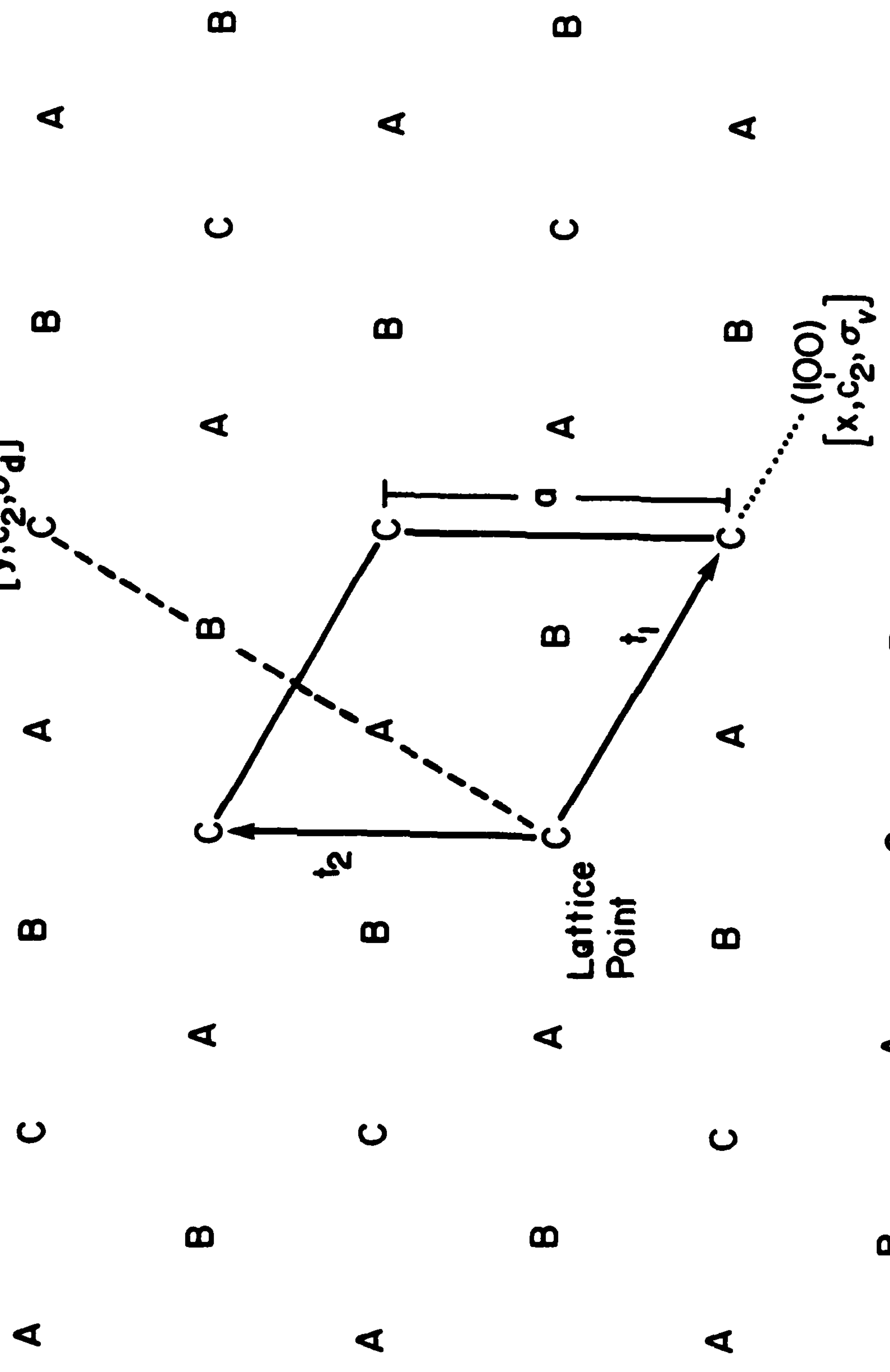

Figure 16. Atomic arrangement in transition metal trihalide or trichalcogenide layered structures.

TABLE 3

CsCl STRUCTURE HALIDES

Compound	a	ε_∞	ε_s	ω_T	ω_L
TlCl	3.84	4.76	31	62	
NH_4Cl	3.87				
TLBr	3.97	5.34			
CsCl	4.11	2.62	7.20	99	165
TlI	4.20		29.6		
CsBr	4.29	2.83	6.51	73	112
CsI	4.56	3.02	5.65	62	85

TABLE 4

ROCKSALT STRUCTURE HALIDES

Compound	a	ε_∞	ε_s	ω_T	ω_L
Li F	4.02	1.93	9.27	307	662
Li H	4.08	3.6	12.9	590	1,120
Na F	4.67	1.75	5.3	239	414
Li Cl	5.14	2.75	11.05	191	662
K F	5.33	1.85	6.05	190	326
LiBr	5.49	3.17	13.2	159	325
AgCl	5.55	4.04	12.3	101	
NaCl	5.64	2.3	5.62	164	264
Rb F	5.63	1.93	6.5	79	
AgBr	5.77	4.62	13.1	79	
NaBr	5.94	2.61	5.99	134	209
LiI	6.00		11.03		
CsF	6.01				
KCL	6.28	2.15	4.68	142	214
NaI	6.46	2.96	6.60	117	209
RbCl	6.54	2.18	4.9	116	173
K Br	6.59	2.35	4.78	113	113
Rb Br	6.87	2.34	4.9	88	127
KI	7.05	2.67	4.94	101	139
RbI	7.33	2.58	5.0	75	103

the sandwich. Only a weak Van der Walls interaction occurs between the anions in adjacent sandwiches. For this reason the layered compounds are attractive in designing materials with modulated physic properties. Even if adjacent sandwiches were comprised of different compounds, rather than true solutions, there should be a low level of interface states.

The arrangement of atoms within any given sheet is hexagonal. The stacking of adjacent sheets in layers that assume a trigonal coordination is ABC, so that a plane taken through the material as shown in Figure 7.2 will contain an atom from each sheet in the structure, resulting in the representations given in Figure 7.3 and 7.4.[9-11] These figures depict the two stacking polytypes assumed by halide compounds, the CdI_2 and $CdBr_2$ structures. Lattice constants for halide compounds with these structures are given in Tables 5 and 6. On the basis of their lattice constants, CdI_2 type systems of interest appear to be $Ti_xV_{1-x}Cl_2$; bromides of Fe-V-Mg-Mn solutions; $Co_xFe_{x-1}I_2$; and iodides of Ti-Ge-Mg-Mn, Ca-Yb-Tm-Pb, and Cd-Zn-Bi-Te solutions. Similarly, $CdBr_2$ structure materials worth looking into are $Zn_xCd_{1-x}Br_2$, and chlorides of Ni-Co-Fe-Mg and Mu-Zn-Cd solutions.

Almost all of the optical measurements on layered compounds have been made at short wavelengths, with a view toward eliciting information on their band structures. Sinha and Mukherjee[12] and Doni and Grosso[13] have made such measurements on PbI_2, which has many stacking polytypes, and an index of refraction of 2.9. Yashiro, et al., reported on the emission spectra of PbI_2,[14] and Ghita, et al, made ellipsometric studies on it.[15] References 16 and 17 report on the phonon spectrum of PbI_2. Kondo and Matsumoto made reflection measurements above 4eV on $CdCl_2$ and $CdBr_2$ crystals,[18] while Srivasta and Bist measured the infrared absorption of CdI_2.[19] Anderson and Lo[20] give the phonon spectra of several layered halides. Many trichlorides also form layered

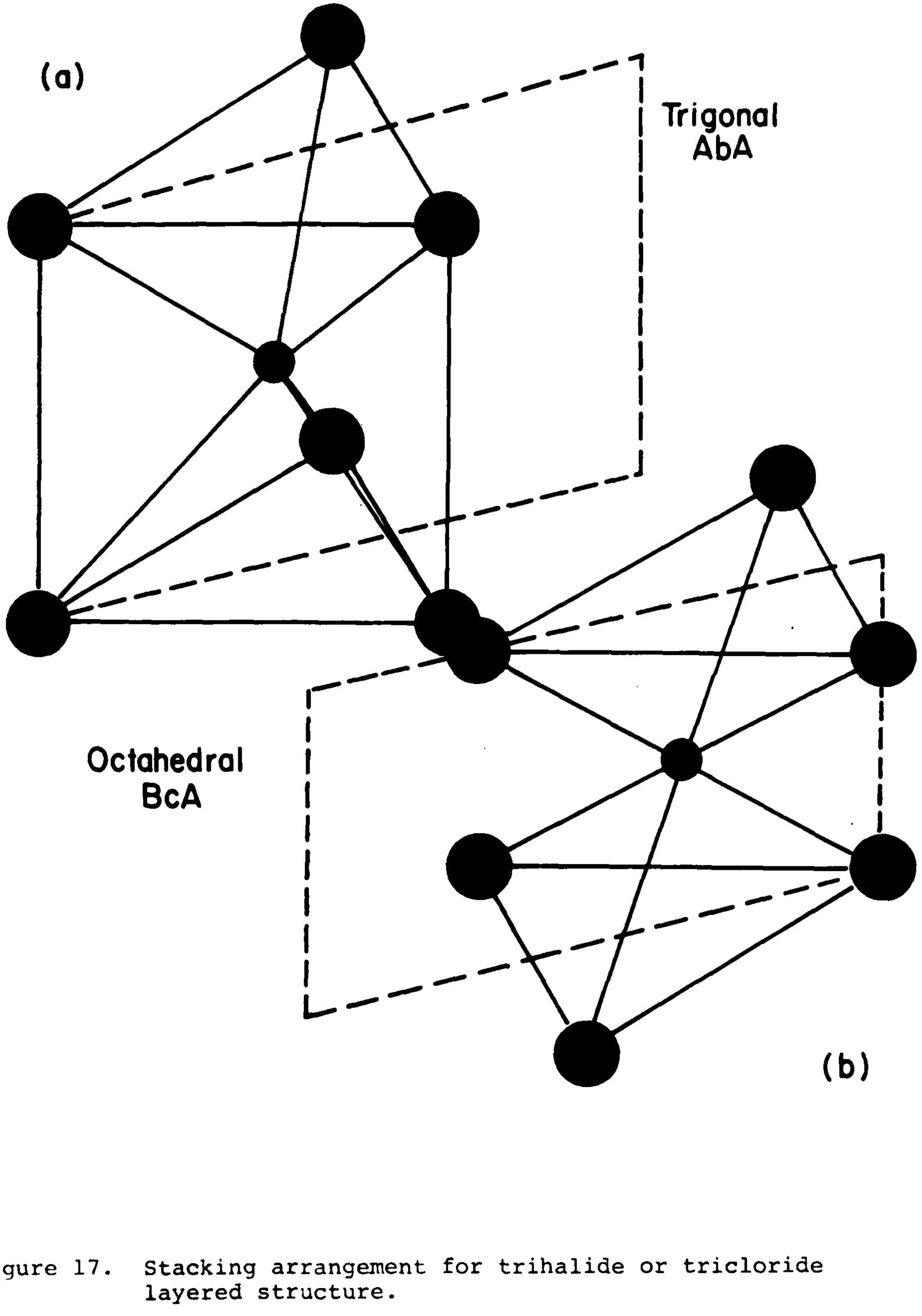

Figure 17. Stacking arrangement for trihalide or tricloride layered structure.

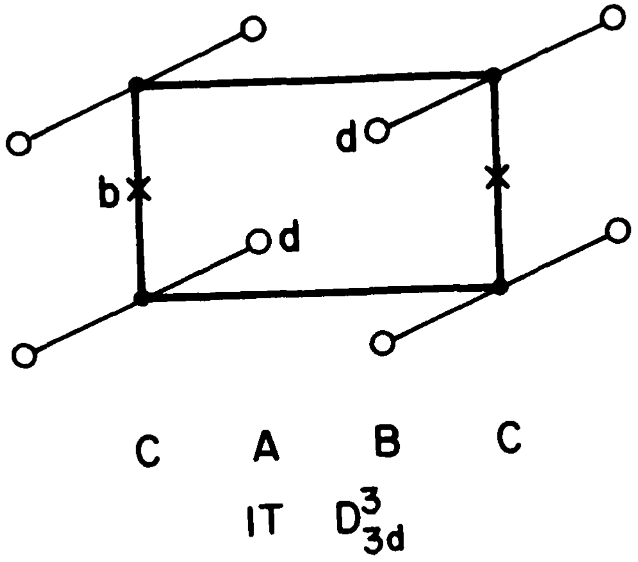

Figure 18. CdI_2 structure stacking polytype.

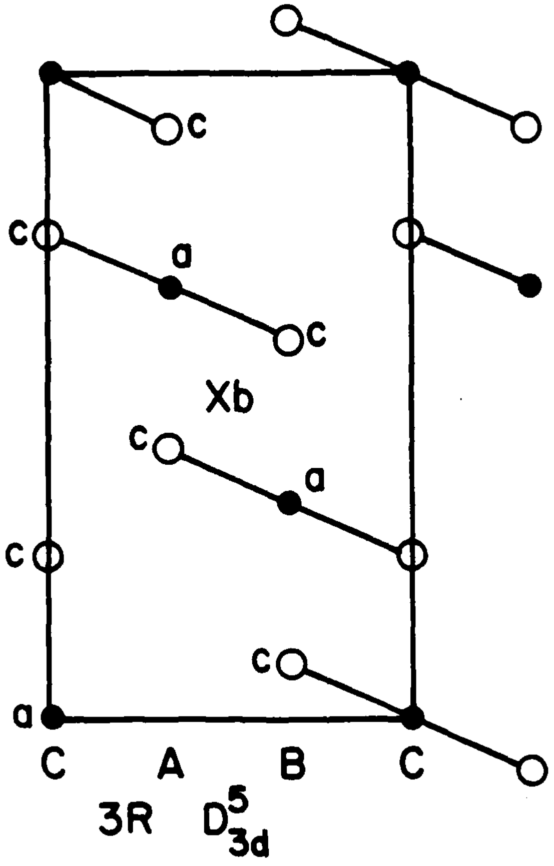

Figure 19. $CdBr_2$ structure stacking polytype.

TABLE 5

CdI_2 STRUCTURE - HALIDES

Compound	a	c
$TiCl_2$	3.561	5.875
VCl_2	3.601	5.835
$TiBr_2$	3.629	6.492
$CoBr_2$	3.68	6.12
$FeBr_2$	3.74	6.17
VBr_2	3.768	6.180
$MgBr_2$	3.81	6.26
$MnBr_2$	3.82	6.19
CoI_2	3.96	6.65
FeI_2	4.04	6.75
TiI_2	4.110	6.820
GeI_2	4.13	6.79
MgI_2	4.14	6.88
MnI_2	4.16	6.82
BiTeBr	4.23	6.47
CdI_2	4.24	6.84
ZnI_2	4.25	6.54
BiTeI	4.31	6.83
CaI_2	4.48	6.96
YbI_2	4.503	6.972
TmI_2	4.520	6.967
PbI_2	4.555	6.977

TABLE 6

$CdBr_2$ STRUCTURE

Compound	a	c
$NiCl_2$	3.543	17.335
$CoCl_2$	3.544	17.430
$FeCl_2$	3.579	17.536
$MgCl_2$	3.596	17.589
$MnCl_2$	3.686	17.470
$NiBr_2$	3.708	18.300
$ZnCl_2$	3.774	17.765
$CdCl_2$	3.854	17.457
NiI_2	3.892	19.634
$ZnBr_2$	3.92	18.73
$CdBr_2$	3.95	18.67
ZnI_2	4.25	21.5
PbI_2	4.54	20.7

compounds. The infrared properties of $TiCl_3$ were studied by Emeis, et. al.[21]

7.3 Oxides

The oxides form a natural group of optical materials, due to their wide band gaps, high melting points, and resistance to chemical attack. There are far too many of them to be given a proper treatment in this paragraph; consequently our discussion will only be cursory. As elsewhere in this section, we will confine our remarks to simple compounds. The simplest system is the Rocksalt structure. There are a large number of oxides in this system, with an almost continuous distribution of lattice constants, as can be seen from Table 7. The most closely matched systems are $Ni_xTi_{1-x}O$, $Nb_xMg_{1-x}O$, and $Pu_xPa_{1-x}O$. The latter systems have a lattice match to within 0.05%. Many of these oxides, especially those of vanadium and titanium, form a series of defect-structure nonstoichiometric compounds. Nonstoichiometric oxides are discussed at length in Sorensen,[22] and will not be dealt with here. We note from the entrees on the dielectric constants in Table 7 that the oxides tend to have somewhat larger dielectric constants than the halides.

The Rutile family is a second collection of familiar oxides. These materials are listed in Table 8, from which we see that the Ge-Mn-Cr, Ta-Sn-Nb, and W_xMo_{1-x} systems are the best possibilities for Rutile-type oxides. As in the case of the dichalcogenides, which we will discuss in paragraph 7.4, the small molybdenum and tungsten cations form dioxides with nearly equal lattice constants. Lattice constants for Table 8 and most of the following tables were obtained primarily from Wyckoff.[23,24] A similar but slightly more complex family of oxides is given in Table 9, which suggests that solutions of Cr-Ga-Rh-Fe with SbO_4, of Nb-Ta with CrO_4, of Sb-V with RhO_4, $Ta_xNb_{1-x}FeO_4$, $Fe_xRb_{1-x}NbO_4$, and $Fe_xRh_{1-x}TaO_4$ are suitable candidate materials for continuously modulated devices.

TABLE 7

ROCKSALT STRUCTURE OXIDES

Compound	a	ε_∞	ε_s
VO	4.062*		
NiO	4.1684†		
TiO	4.1766*		
NbO	4.2097		
MgO	4.2112	2.95	9.65
CoO	4.2667†		
TaO	4.43		
MnO	4.4448	4.8	
ZrO	4.62		
CdO	4.6953	5.40	
CaO	4.8105	3.33	
YbO	4.86		
PuO	4.959		
PaO	4.961		
SmO	4.9883		
NpO	5.01		
EuO	5.1439		
SrO	5.1602	3.46	

*V and Ti tend to form a series of non-stochiometric oxides

†

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BASED ON AN ANALY..(U) UNIVERSAL ENERGY SYSTEMS INC
DAYTON OH R J BECKER JAN 86 AFWAL-TR-85-4129
UNCLASSIFIED F33615-82-C-5001 F/G 20/6 NL

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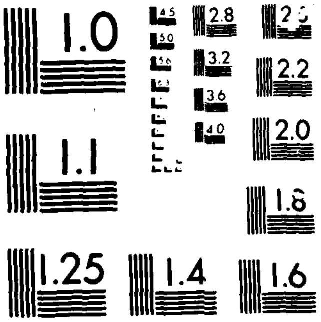

MICROCOP CHART

TABLE 8

CASSITERITE OR RUTILE STRUCTURE OXIDES

Compound	a	c	n
GeO_2	4.395	2.859	1.6525
MnO_2	4.396	2.871	
CrO_2	4.41	2.91	
IrO_2	4.49	3.14	†
OsO_2	4.51	3.11	
RuO_2	4.51	3.19	†
TiO_2	4.594	2.958*	2.3 - 2.7
TaO_2	4.709	3.065	
SnO_2	4.737	3.186	
NbO_2	4.77	2.96	
TeO_2	4.79	3.77	
WO_2	4.86	2.77	
MoO_2	4.86	2.79	
PbO_2	4.946	3.379	

* Ti tends to form a system of nonstochiometric oxides.

† Metallic

TABLE 9

RMO_4 ARRANGEMENT

Compound	a	c
$AlSbO_4$	4.510	2.961
$CrSbO_4$	4.577	3.042
$GaSbO_4$	4.59	3.03
$RhSbO_4$	4.601	3.100
$RhVO_4$	4.607	2.923
$FeSbO_4$	4.623	3.011
$CrTaO_4$	4.626	3.009
$CrNbO_4$	4.635	3.005
$FeTaO_4$	4.672	3.042
FeNbO4	4.68	3.05
$RhTaO_4$	4.684	3.020
$RhNbO_4$	4.686	3.014

The rutile materials tend to exhibit high dispersion. Studies of titanium dioxide films have been made by Cherepanova and Titova,[25,26] Schiller et al.,[27] Joseph and Gagnaire[28] and Perney et al.[29] The index of refraction of TiO_2 can vary by 10% depending on the preparation procedure. The absorption coefficient, κ, can be reduced to 10^{-4} with proper care. It can also be raised very high with the addition of impurities such as copper.[30] Gagnaire and Joseph also studied the Ti/TiO_2 system.[31] Samara and Peercy measured the pressure and temperature dependence of ε_s for rutile.[32] The optical properties of the metals RuO_2 and IrO_2 were studied by Goel, et al.[33] while the Raman spectrum of TeO_2 was taken by Pine and Dresselhaus.[34] The optical properties of SnO_2 are discussed in references 35-37.

In addition to the Rutile structure, MoO_2 and WO_2 can also have a monoclinic structure closely resembling the Rutile structure. Since MoO_2 and WO_2 can occur in more than one phase, the attractiveness of the $Mo_xW_{1-x}O_2$ system is considerably reduced. This consideration is accentuated by the implications of a monoclinic structure for the anisotropy of the dielectric constant. The dioxides of Re and Tc also have this monoclinic structure. The lattice parameters for these materials are given in Table 10, along with those for (monoclinic) VO_2, which has a closely related structure. Since V easily forms a series of nonstoichiometric oxides and VO_2 is not only imperfectly matched to the crystal structure of other oxides, but undergoes a metal-to-insulator phase transition at 68 C, it is not a promising compound. We conclude that although the dioxides of a Re, W, and Mo are closely matched, the materials listed in Table 10 are not good candidates for continuously modulated devices. Studies on tungston oxide films are reported in References 38-40.

The optical properties of VO_2 were measured by Mokerov and Begishev as a function of temperature.[41] Vanadium oxide films

TABLE 10

MONOCLINIC DIOXIDES

Compound	a	b	c	n
VO_2	5.743	4.517	5.375	2.81
TcO_2	5.53	4.79	5.53	
ReO_2	5.562	4.838	5.561	
WO_2	5.565	4.892	5.650	
MoO_2	5.584	4.842	5.608	

were studied by Gur'yanov and Terukov.[42] Other vanadium oxides were studied by Mokerov et al.,[43] Mokerov and Ryabinin,[44] and Van Hove et.al.[45]

Many dioxides have the cubic fluorite structure; these are listed in Table 11. From Table 11 we see that $Cm_xAm_{1-x}O_2$, $Pu_xCe/_{1-x}O_2$, and UO_2PrO_2, should form continuous solutions, with lattice matchings of better than 0.3%. Taguchi et al.,[46] studied ZiO_2 films, and found that the dielectric constant varied from 1.72 to 2.0, depending on the gas pressure at which the films were formed.

Several other oxides were investigated in our literature search, none of which appears promising for device applications. Tanaka[47] gives curves for several low-index, high-absorbance oxides, which are listed in Table 12. The best of these is MnO, which has the rocksalt structure. The high absorbance of one of these compounds, Re_3O_4, was also studied by Schlegal et al.[48,49] High absorbance was also studied for Co impurities in Al_2O_3 by Niklasson and Grangvist.[50]

The tetragonol materials, $DyVO_4$ and $DyAsO_4$ are questionable because their refractive indices are low and very similar.[51] The indices for $DyVO_4$ are 2.02 and 2.25; for $DyAsO_4$ they are 1.84 and 1.96. Feldman et al. reported on the Faraday rotation exhibited by $Bi_{12}GeO_{20}$, $Bi_{12}SiO_{20}$, $Bi_{12}TiO_{20}$, ZnO, Bi_2O_3, and Ga_2O_3.[52] These materials would be useful in certain cases due to their magneto-optic properties. The dielectric constants of $Bi_{12}SiO_{20}$ were investigated by Reza et al.[53] Thin films of Bi_2O_3 contain a high density of voids but the refractive index of about 2.55 is not sensitive to variations in stoichiometry.[54]

The remainder of our literature search pertained to materials commonly used in the glassy state. Hing investigated losses in sintered alumina.[55] He found that both Mg and Ca,

TABLE 11

CUBIC FLUORITE-STRUCTURE OXIDES

Compound	a	n
ZrO_2	5.07	1.72 - 2.0
HfO_2	5.115	4.0
TbO_2	5.220	
CmO_2	5.372	
AmO_2	5.376	
PuO_2	5.3960	
CeO_2	5.4110	
UO_2	5.4682	
PrO_2	5.4694	
PaO_2	5.505	
ThO_2	5.5997	

TABLE 12

HIGH-ABSORBANCE OXIDES

Compound	n	k
MnO	2.2	small
Mn_3O_4	2.4	0.2
ZnO	2.0	0.2
TiO_2	2.7	0.3
Fe_2O_3	2.8	0.4
Mn_2O_3	2.7	0.5
Cu_2O	2.7	0.5
CuO	2.4	0.5
Fe_3O_4	2.2	0.5
V_2O_5	2.1	0.5
Co_3O_4	1.4	0.8

which are often used to control sintering, segregated to the grain boundaries. High absorption occurs in sintered alumina due to residual porosity, grain-boundary contamination, and second-phase scattering. Best results were obtained using MgF as a dopant. The effect of stoichiometry on a common companion of alumina in glasses, SiO_2, was reported by Zuther, et al. who studied the glass system Ga_2O_3-GeO_2-As_2O_5.[56] The refractive indices of the monoclinic materials $PbGeO_3$ and $PbSiO_3$ were measured by Sugi et al,[57] and are given in Table 13. These anisotropic materials have similar refractive indices with high dispersion. The refractive indices of oxide films on Ge and GaAs are reported respectively by Nazarenko and Rastrenenko[58] and Umeno, et al.[59] Finally, Ovcharenko and Yakhkind looked at several oxide additives in tellurite glasses.[60] Their results are presented in Table 14, which gives an extrapolation of the effective indices of these additives to a 100% concentration. The refractive index of TeO_2-BaO is 2.0976, and that of TeO_2-WO_3 is 2.1939. We take the coexistence of oxides and tellurides as a transition to our next paragraph, the chalcogenides.

7.4 Chalcogenides

The II/VI compounds are a well understood and well developed class of materials in which we make the transition from oxides to chalcogenides. This is because ZnO and BeO have the wurtzite structure, although their disparate respective lattice constants of 3.25 and 2.69 angstroms make them unattractive candidates for a solute system, and because the rocksalt structure contains both oxides and chalcogenides. The wurtzite compounds are presented in Table 15, and the rocksalt structured chalcogenides are given in Table 16. Copper halides are also listed in Table 15. None of the wurtzite systems appears attractive for low-defect solid solutions, due to the incompatibility of their lattice parameters. The same comment applies to the rocksalt structure chalcogenides.

TABLE 13

$PbGeO_3$ and $PbSiO_3$

	$PbGeO_3$	$PbSiO_3$
a	11.57	
b	7.32	
c	12.62	
n_x*	2.0337	1.947
n_y*	2.0411	1.961
n_x*	2.0506	1.968

*Taken at 579.1 nm. These materials have high dispersion.

TABLE 14

OXIDES IN TELLURITE GLASSES

Additive	n	
	TeO_2-BaO	TeO_2WO_3
La_2O_3	1.63	1.73
Gd_2O_3	1.62	1.62
Y_2O_3		1.56
CdO	1.57	1.86
Sc_2O_3	1.48	1.51
ZnO	1.61	1.63
Ga_2O_3		1.48
As_2O_3	1.82	1.82

TABLE 15

WURTZITE STRUCTURE

Compound	a	c	ε_∞	ω_T	ω_L
Halides					
CuH	2.893	4.614			
CuCl	3.91	6.42			
CuBr	4.06	6.66	4.4		
CuI	4.31	7.09			
AgI	4.580	7.494			
Oxides					
BeO	2.698	4.380	3.0		
ZnO	3.250	5.207	3.7	381 407	574 583
Chalcogenides					
ZnS	3.811	6.234			
MnS	3.976	6.432			
ZnSe	3.98	6.53	5.9		
MnTe	4.087	6.701			
MnSe	4.12	6.72			
CdS	4.135	6.749	5.6	228 235	305
ZnTe	4.27	6.99			
CdSe	4.30	7.02	6.2	171	214
MgTe	4.52	7.33			

TABLE 16

ROCKSALT STRUCTURE CHALCOGENIDES

Compound	a	ε_∞	ε_s
MnS	5.22		
CdS	5.516	5.30	10
CaS	5.689		6.67
PbS	5.9436	17.2	205
SuSe	6.020	22.9	
PbSe	6.124		280
SnTe	6.313	45.0	
PbTe	6.454	32.8	

Another reason for passing over these materials is that ZnS, Zns-Se, CdS, MnS, and MnSe can assume both the wurtzite and zincblende structures. CdS and MnS can have the rocksalt structure as well. Furthermore, many II/VI materials do not resist moisture well.

Among the zincblende structure chalcogenides, $Hg_xCd_{1-x}Te$ appears to be the most likely candidate system, as can be seen from Table 17. This system is especially attractive due to the high and very different dielectric constants for HgTe and CdTe respectively of 14.0 and 7.3. In fact, $Hg_xCd_{1-x}Te$ is known to form a continuous solution as a function of x. The x value must be kept above 0.15 to maintain a bandgap. The reflection spectrum of $Hg_{.75}Cd_{.25}Te$ was taken by Kavalyauskas et al.[61] These authors obtained a dielectric constant of 12 for this solution. The refractive index of ZnS as a function of temperature is given by Thompson et al.[62] Solutions of cubic $CdSe_{1-x}$, $Cd_{1-x}Mn_xSe$, and ZnS_xSe_{1-x} were investigated respectively by Kainthla et al.[63] Antoszewski and Pecold,[64] and by Mach et al.[65] Klassen and Ossipyan looked at the effect of dislocations on CdS and CdSe. They found that the inhomogeneities caused by dislocations caused focusing and channeling of light passing through these materials.[66]

Many transition metal/dichalcogenide compounds take the pyrite structure (see Table 18). From Table 18 we see that Ru_xOs_{1-x} solutions with either S, Se, or Te should make excellent lattice matches. Infrared measurements on several pyrites were reported by Anastassakis and Perry.[67] Verble and Humphrey[68] measured the infrared and Raman spectra of MnS_2, and Ushioda reported on Raman measurements on FeS_2.[69]

One reason why the chalcogenides can be interesting is that sulfur and selenium have similar crystal radii, of 1.84 and 1.98 angstroms respectively, so that several solutions of S_xSe_{1-x} are

TABLE 17

ZINCBLENDE OR SPHALERITE STRUCTURE CHALCOGENIDES

Compound	a	ε_∞	ε_S	ω_T	ω_L
BeS	4.85				
BeSe	5.07				
ZnS	5.409	5.14	8.0	282	352
BeTe	5.54				
MnS	5.600				
ZnSe	5.668	5.90	8.3-9.1	207	246
MnSe	5.82				
CdS	5.818	5.63			3
HgS	5.85		30.6		
HgSe	6.084		25.6		
ZnTe	6.089	7.28	10	178	206
CdSe	6.16	6.38			
HgTe	6.429	14.0			
CdTe	6.480	7.3		140	171
CuCl	5.406	3.6	7.3	155	198
CuBr	5.690	4.4			
CuI	6.043	5.2			

TABLE 18

PYRITE STRUCTURE CHALCOGENIDES

Compound	a	ε_∞
FeS_2	5.407	21.3
CoS_2	5.52	
RhS_2	5.574	
RuS_2	5.59	
OsS_2	5.608	
$CoSe_2$	5.859	
$RuSe_2$	5.921	
$OsSe_2$	5.933	
$NiSe_2$	5.960	
$RhSe_2$	5.99 - 6.00	
MnS_2	6.101	6.07-6.14
$RuTe_2$	6.360	
$OsTe_2$	6.369	
$IrTe_{2+}$	6.411	
$RhTe_2$	6.441	

known. In addition, some chalcogenides have large dielectric constants. However, chalcogenides tend to have narrow bandgaps, and are best suited for use in the infrared. Like the halides, many chalcogenides form layered compounds with transition metals.[70] These materials are discussed at length in Wieting and Schluter.[71] The materials are most commonly grown by halogen vapor transport.[72] Often it is possible to grow large single crystals, one exception being WS_2. Many of these layered compounds are metals, but several are semiconductors. One of the better known layered structures occurs for GaS and GaSe. Data on these compounds are given in Table 19, where N refers to the number of layers within a unit cell. We see that GaS and GaSe do not have either commensurate lattice parameters or particularly interesting refractive indices. GaSe is an electro-optic material; its electro-optic properties have been measured by Sokolov and Subashiev.[73] The temperature dependence of the refractive index of GaSe was investigated by Antonioli, et al.[74] The dispersion in GaSe is very high, with a refractive index that varies from about 2.73 at 0.5 eV to 3.10 at 2.5 eV.[74] Reflectivity measurements on GaS_xSe_{1-x} crystals are presented in Reference 75. Other optical measurements on GaSe are given in References 76-80.

The most common layered structure formed by the transition metal dichalcogenides is the CdI_2 structure shown in Figure 7.1a. Many of these compounds are metals, but except for $SnSe_2$, the materials of Table 20 are semiconductors. We see from Table 20 that solutions of Hf/Sn/Zr in either sulfur or selenium are possibilities for high-index devices with a potential for modulation of over 30%. The sulphides are particularly attractive, since they have wider bandgaps, a much closer (1%) match in lattice constants, and do not contain any metals. Infrared reflectance measurement on many of these compounds were made by Lucovsky et al.[81] Optical and U.V. measurements on $SnSe_2$ and

TABLE 19

GaS STRUCTURE

Compound	a	c	N	n
GaS	3.585	15.50	4	3.0
GaSe	3.746	23.910	6	2.7
InSe	4.05	16.93	4	

TABLE 20

CdI_2 STRUCTURE - CHALCOGENIDES

Compound	a	c	ε_∞
HfS_2	3.635	5.837	6.20
SnS_2	3.639	5.868	9.5
ZrS_2	3.662	5.813	9.23
SnSSe	3.716	6.050	
$HfSe_2$	3.748	6.159	8.05
$ZrSe_2$	3.771	6.138-.149	
$SnSe_2$	3.811	6.137	11

SnS_2 were made by Bertrand et al.[82] Other papers on the optical properties of SnS_2 and $SnSe_2$ are given in references 83 and 84. Isomaki and Boehm have made calculations on the dielectric properties of ZrS_2.[85]

The best known transition metal dichalcogenide, MoS_2, belongs to the octehedrally coordinated family listed in Table 21, and depicted in Figure 7.1b. These materials have large dielectric constants (7-24), albeit narrow bandgaps. As in the case of the 1T-CdI_2 materials, we find that a match of lattice constants separates the Mo_xW_{1-x} solutions into sulphides and selenides. Of these, the sulphides are harder to grow.

Beal and Liang have made reflectivity measurements on WSe_2 and WS_2.[86] The optical properties of $MoSe_2$, which is relatively easy to grow, were measured by Evans and Hazelwood.[87] Other relevant papers are references 88 and 89. We note that many transition metal trichalcogenides also take layered structures. Zwick, et al. made Raman measurements on ZrS_3, $ZrSe_3$, $ZrTe_3$, and $HfSe_3$.[90] The infrared spectrum of HfS_3 was measured by Jandl and Deslandes.[91]

The system $Bi_2Te_{1-x}Se_x$ also has a layered structure. It has a very high dielectric constant (20-40) in the region between 2 and 10 μm, where it has an extinction coefficient of less than one μm.[92] Orpiment, Hs_2S_3, and its companion, As_2Se_3, may crystallize in a layered form, or can form glasses. Most work on these materials has been done on the glass phase. These glasses have good mechanical strength and chemical stability. However, their range of refractive indices is small (n varies from 2.4 to 2.7), and their ability to form both a glass and a crystalline phase suggests that scattering from defects may be a problem. Butterfield[93] started the optical properties of 40 thin films of these glasses. He attributed the dominant scattering mechanism to void and oxygen impurities. Kanchiev and Kokorina concur

TABLE 21

MOLYBDENITE STRUCTURE

Compound	a	c	ε_∞
MoS_2	3.16	12.30	10 (2.2μm)
WS_2	3.15	12.36	7-8
$MoSe_2$	3.29	12.93	24
WSe_2	3.29	12.97	7.3

that oxygen impurities are a serious problem, as is water.[94] They suggest distillation as a means of removing these impurities. Young[95,96] finds that the absorption and reflectivity of As_2S_3 films depend on surface preparation, especially the finish and the temperature at which the films were deposited. Other papers on the optical properties of these glasses are given in references 97-107. GeS_2 can also take both a glassy and a crystalline form, and is sometimes used to form glasses and As_2S_3. Raman studies on GeS_2 have been made by Nemanich.[107,108] The single sulphides and selenides of Ge and Sn have an orthorhombic structure (Table 22). These materials do not appear to be well suited for continuously modulated optical devices. Their optical properties are reported in references 109-116. Miscellaneous references on chalcogenide compounds are given in references 117-121.

Our remaining structure for chalcogenide compounds is the chalcopyrite structure. This structure is shared by some arsenic compounds and thus forms a bridge with the Group V materials. The chalcopyrites, listed in Table 23, are birefringent and difficult to grow in large crystals. From Table 23 we see that there are four closely matched systems, all of which contain either Cu or Ag, and most of which contain either Al or Ga. Most of these materials are selenides. Of the four systems, $CuAl_xGa_{1-x}S_2$, $CuAl_xGa_{1-x}Se_2$, have very closely matched lattice parameters. The $In(CuSe_2)_x(AgS_2)_{1-x}$ and $Al(AgSe_2)_x(CuTe_2)_{1-x}$ systems are likely to form localized compounds such as $InCuS_2$ or $AlCuSe_2$, which would have dissimilar lattice parameters. The Raman and infrared spectra of $AgGaS_2$ was taken by Holah et al.[122] $AgGaS_2$ has a direct band gap of 2.75 eV, and a large nonlinear optical coefficient.[123] Many chalcopyrites also take the zinc-blend structure. The $(CuInSe_2)_{1-x}$ - $(ZZnSe)_x$ system was studied by Gan et al., in this context.[124] The reflectivity of a number of chalcopyrites was measured by Rife et al.[125]

TABLE 22

GeSe STRUCTURE

Compound	a	b	c
GeSe	4.40	11.82	3.85
SnS	4.33	11.18	3.98
GeS	4.30	10.44	3.65
SnSe	4.46	11.57	4.19
$PbSnS_2$	4.23	11.42	4.09

TABLE 23

CHALCOPYRITES

COMPOUND	a	c
$CuAlS_2$	5.312	10.42
$CuGaS_2$	5.349	10.47
$CuInS_2$	5.517	11.06
$CuTlS_2$	5.580	11.17
$CuAlSe_2$	5.606	10.90
$CuGaSe_2$	5.607	10.99
$ZnSiAs_2$	5.608	10.89
$AgFeS_2$	5.66	10.30
$ZnGeAs_2$	5.670	11.153
$AgAlS_2$	5.695	10.26
$AgGaS_2$	5.743	10.26
$CuInSe_2$	5.773	11.55
$AgInS_2$	5.816	11.17
$CuTlSe_2$	5.832	11.63
$CdGeAs_2$	9.942	11.224
$AgAlSe_2$	5.956	10.75
$CuAlTe_2$	5.964	11.78
$AgGaSe_2$	5.973	10.88
$CuGaTe_2$	5.994	11.91
$AgInSe_2$	6.090	11.67
$CdSnAs_2$	6.092	11.922
$CuInTe_2$	6.167	12.34
$AgGaTe_2$	6.288	11.94
$AgInTe_2$	6.406	12.56

7.5 Group V Compounds

The group V materials have strongly covalent bonds, and in general exhibit narrow bandgaps. Consequently they are of interest primarily for infrared devices. The nitrogen compounds tend to have bond lengths that are not well matched to those of P, As, or Sb, so we will concentrate our attention on the latter chemicals, and defer a discussion of nitrogen compounds to the end of this paragraph.

By far the most well developed and most commonly used group V materials are the III-V compounds with the zincblende structure. Simply by virtue of current materials processing capability, these compounds deserve attention, and are listed in Table 24, in which are included the closely related materials Si and Ge. These materials do suffer from generally narrow bandgaps and low melting temperatures. However, they can be grown on a large scale with a very low level of defects. From Table 24 we see that an Al_xGa_{1-x} solution with either P, As, or Sb will give a good lattice match, albeit with a variation in dielectic constant of only about 20%. Continuous modulation of these materials should reduce the bandbending associated with interfaces.[126] It thus seems that these materials are attractive for narrow-band ignition filters, provided that input power levels are not too high. References 127-130 concern the optical properties of some of these materials.

Our final group of materials are the nitrides with the ZnO structure (see Table 25). We expect these nitrides to have wider bandagaps and higher melting points than the zincblende compounds of Table 24. It appears that the $Ga_xAl_{1-x}N$ and $Nb_xTa_{1-x}N$ systems are good candidates for optical devices.

TABLE 24

III/V COMPOUNDS - ZINCBLENDE STRUCTURE

COMPOUND	a	n		ε_∞	ε_S	ω_T (cm^{-1})
		.6	5			
SiC	4.348			6.7	10.2	793
BP	4.538				10.2	
Si	5.4307		3.5		11.7	520
GaP	5.4505	3.46	2.94	8.5	10.18	366
AlP	5.451			7.6		440
AlAs	5.62			9.0		361
GaAs	5.6537			10.9	13.13	269
Ge	5.6574		4.016	16	15.8	309
InP	5.8687	3.44	3.08	9.6	12.37	304
InAs	6.036	4.17	3.46	12.3	14.6	219
GaSb	6.118		3.824	14.4	15.7	230
AlSb	6.1347	4.24		10.2	11.2	319
InSb	6.478			15.6	17.88	180

TABLE 25

ZnO STRUCTURE NITRIDES

COMPOUND	a	c	ε_∞	ω_T
AlN	3.111	4.978	4.8	622
GaN	3.180	5.166	5.8	
InN	3.533	5.693		
NbN	3.017	5.580		
TaN	3.05	4.94		

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8. CONCLUSION

We now present the conclusions resulting from our literature survey and preliminary analysis. Although he has not definitively proved all of these conclusions, the author believes that they are valid over sufficiently general conditions to warrant their entry in this report. We assert that:

- Stop and pass bands will be formed whenever the susceptibility is periodically modulated. In fact a series of such bands will occur as a function of the wave frequency. The band structure will become more sharply defined as the number of repeat regions, or unit cells, increases, and as the medium approaches absolute periodicity. It is likely that the sharpness of the band edges will be enhanced if the imaginary part of the material susceptance is minimized.

- The centers of successive stop bands occur at wavelengths for which the optical depth of the medium taken over a unit cell distance is an integral number of half wavelengths, i.e., the phase angle is equal to π, or

$$k_o \int_o^d dx\ n(x) = \pi \quad . \tag{8.1}$$

Thus the location of the gaps, or stop bands is determined primarily by the dimension of the unit cell, d, and the mean value of the refractive index, $\overline{n}(x)$, rather than the shape of the modulation profile.

- The width of the band gaps, or stop bands increases as the relative modulation in the refractive index, $\Delta n/\overline{n}$, increases. For small modulations, in most cases the widths of stop bands of a given order are roughly proportional to components of the Fourier transform of the modulation profile of similar order.

- The degree of attenuation of a wave with a frequency within a stop band increases toward the middle of the band. The amount of attenuation is proportional to $\Delta n/\bar{n}$. If the number of repeat units (unit cells) in the filter is sufficiently large, such a wave will not propagate through the filter at all, it will be totally stopped. The attenuation of the wave is not due to absorption, it is due to reflection, i.e., the stop bands correspond to reflection bands.

- Complex modulation profiles in the medium susceptance will lead to "band splitting"--the formation of new stop bands within what would otherwise be pass bands. Consequently several stop bands can be located at arbitrary frequencies within say, one octave of the first stop band by appropriate design of the modulation profile. The locations and widths of the various stop bands will be related to the filter parameters in the same manner as for a single stop band. If it is desired to locate stop bands at arbitrary intervals over a multioctave region, then it will probably be necessary to put up with additional "ghost" stop bands.

- As $\bar{n}$ increases, the acceptance angle for the filter will also increase.

- Unless performance is desired over many octaves, there is no apparent reason to favor one type of unit length modulation profile (e.g., a step function as a sinusoidal, parabolic, or Gaussian profile) over another. Details of the modulation profile only become significant in the upper level stop, or reflection bands. There may be reasons based on materials for choosing a given type of modulation profile. For example, it may be that impurities will aggregate at discontinuities. However, our analysis in Paragraph 2.2 suggests that even if such an aggregation were to occur, it would not affect the amount of absorption in most cases. Some effect might be discernable at stop bands.

In addition, we have made a brief preliminary survey of possible materials for graded-index optical devices. In our analysis we assumed that a minimization of absorption was paramount, and accordingly sought systems that offered a hope of achieving a low density of defects and an infrared spectrum relatively free of absorption bands. This implied a choice of optical materials with simple molecular formulas, materials that crystallize with identical structures and closely matched lattice parameters, and materials that are known to crystallize in only one form. In particular, we noted that many potential candidate materials are layered compounds. It may be possible to use layered materials with dissimilar chemical formulas in adjacent layers without introducing serious problems with interface states.

8.1 Comments

The author is confident that an analytic description of a filter behavior similar to that discussed in Sections 3-6 can be extended to complex susceptibilities and three-dimensional systems. Similar problems have been treated in three dimensions in band theory, lattice dynamics, and the description of microwave components. Step function modulations are the easiest to analyze because the solutions are in terms of sines and cosines, which are familiar, and can often be manipulated into compact expressions. The analysis of a Rugate filter is much less tractable. However, in many cases of interest, such as sinusoidal modulation, closed form solutions should be obtainable. Indeed, solutions to the Mathieu problem have been known for over half a century.

Commonly, continuously modulated filters are approximated in manufacture by stacking together a large number of very thin layers, with flat index profiles across each layer and sharp discontinuities between layers. Our analysis suggests that the merit of this procedure is at best moot. This practice will indeed give a reasonable approximation of an arbitrary index profile over a limited (one or two octave) frequency range. However, it introduces a very large number of discontinuities. If these discontinuities do, in fact, result in deterioration of the material properties, then these discontinuities are self defeating. They will also affect the structure of high-order bands. Therefore if the higher-order band structure is important, the use of thin layers will interfere with these upper-level bands.

We note that both the width and the degree of attenuation or reflection in the stop or reflection bands scales as $\Delta n/\bar{n}$. This creates difficulties if notch filters are desired. It appears that the primary way out of this dilemma is to build a filter with many repeat distances, i.e., a very long filter. It may also be possible to achieve some design freedom by prescribing profiles that have narrow potential wells (regions of large susceptibility) separated by relatively wide distances.

8.2 Implications and Suggestions

On the basis of this interim survey the author concludes that the choice of optimum filter materials and manufacturing should be dominated by materials and manufacturing questions rather than by filter design criteria. The primary concern should be to minimize intrinsic losses. This can be achieved by selecting materials whose imaginary component of the refractive index, n_i, is small compared to the real component, n_r, and by minimizing local inhomogeneities which will add to losses, as described in Paragraph 2.2. The second criteria should be to select a material that is immune to intense levels of signal energy. This implies a low variation of $n(x)$ with temperature, and a high melting or phase transition temperature. Comments on nonlinear susceptibilities are beyond the scope of this report.

In general, it will be desirable to adjust the widths of the stop or reflection bands and to create multiple stop bands at arbitrary frequencies. This will require tailor-made refraction indices, which are achieved by appropriate solid solutions. If inhomogeneities in the resulting material are to be minimized, the constituents of the solution should be as compatible (mutually soluble) as possible. This suggests similar structures, chemical compositions, and bond lengths.

In summary, we believe that optimum materials should have the following properties:

- $n_i << n_r$
- Amenability to manufacture with a low concentration of defects
- $dn/dT \rightarrow 0$
- A high phase transition temperature
- Good solubility with other materials possessing a similar structure but as different a refractive index as possible.

This interim report is by its very nature incomplete. If we are to obtain a reasonably complete analytic picture of maximum filter design, several steps should be undertaken. We need to make analytic calculations of the dependence of the imaginary part of the wavenumber, k_i, and the reflection bandwidth, $\Delta\omega$ on the relative modulation depth, $\Delta n/\overline{n}$. These calculations should be made for both the Kronig-Penney and the Mathieu problems, and the respective results should be compared. The analytic calculations should be augmented by numerical calculations, and should be extended to include multiply periodic filters. We should also make numerical comparisons between the Kronig-Penney and the Mathieu contours in regard to their higher-order band structure and the side lobes in their reflection bands.

We should extend our calculation to include complex susceptibilities, including both analytic and numerical work. Formulations should be given for additional profiles, e.g., as sawtooth and parabolic profiles. In particular, we should investigate the application of a Kramers-Kronig analysis to a Bragg filter. The Kramers-Kronig relation is based solely upon causality. Therefore it is reasonable to assume that it will apply to the filters in question. However, since we get stop bands even with ideal materials that have purely real susceptibilities, the applicability of a Kramers-Kronig analysis is not immediately obvious. Assuming that it does apply, it would be very useful both in filter design and in reducing data on filters.

Finally, our analytic formulations should be extended to three dimensions, particularly for the case of the Mathieu problem. Such calculations can most readily be made in Cartesian coordinates, but calculations in a cylindrical coordinate system should also be attempted. If time permits, an analytic treatment of the effect of terminations and interfaces should also be made.

APPENDIX A

MATHEMATICAL UNDERPINNINGS OF WAVE PROPAGATION IN PERIODIC MEDIA

In this appendix we derive some of the equations which form a basis for the discussion of Section 3. The fundamental property that facilitates the description of this problem is that the waves obey a second-order equation of motion,

$$\psi'' + f(x)\,\psi = 0 \quad , \qquad (A.1)$$

in which no first derivative term appears. The second property is that the response of the media to the wave is periodic along the path of the wave. No other properties of the system need to be involved in our discussion. Consequently our remarks apply to many fields other than optics, including acoustics, lattice vibrations, transmission line theory, waveguide theory, and the band theory of solids. In Section 3 we use

$$f(x) = k_o^2 n^2(x) = k_o^2 \varepsilon(x) = k^2(x) \quad . \qquad (A.2)$$

A.1 Form for Transfer Matrix Elements

A second-order differential equation will have two independent solutions for a given set of parameters (e.g., k and ω). Let these be ϕ_1 and ϕ_2. Then, from Equation (A.1),

$$\phi_1\phi_2'' = - f(x)\,\phi_1\phi_2 \qquad (A.3)$$

and

$$\phi_2\phi_1'' = - f(x)\,\phi_1\phi_2 \ . \qquad (A.4)$$

Subtracting (A.4) from (A.3) we have

$$\phi_1\phi_2'' - \phi_2\phi_1' = 0 \quad . \qquad (A.5)$$

This is a key result, which as we see, stems from the form of (A.1). Now

$$\frac{d}{dx}\left(\phi_1\phi_2' - \phi_2\phi_1'\right) = \phi_1\phi_2'' + \phi_1'\phi_2' - \phi_2\phi_1'' - \phi_2'\phi_1' \quad . \qquad (A.6)$$

Consequently, we find

$$\frac{d}{dx}\left(\phi_1\phi_2' - \phi_2\phi_1'\right) = 0 \quad , \qquad (A.7)$$

or

$$\phi_1\phi_2' - \phi_2\phi_1' = \text{constant} \quad . \qquad (A.8)$$

The quantity in the l.h.s. of (A.8) is known as the Wronskian for (A.1). The critical point is that the Wronskian is independent of the argument of ϕ_1 and ϕ_2, as long as they are taken at the same point. Note that if we had an equation of the form

$$\psi'' + \gamma(x)\psi' + f(x)\,\psi = 0 \quad , \qquad (A.9)$$

we would obtain the result

$$\phi_1\phi_2' - \phi_2\phi_1' = \exp\left[-\int\gamma(x)dx\right] \quad . \qquad (A.10)$$

We would need to use (A.10) instead of (A.8) in regard to the full wave Equations (4.1) - (4.4).

We are now in a position to derive the expressions for the matrix elements Equations (3.17) - (3.21). We begin with a general solution to (A.1), which is a linear combination of the independent solutions ϕ_1 and ϕ_2:

$$\psi = c_1\phi_1 + c_2\phi_2 \quad . \qquad (A.11)$$

Differentiation of (A.11) yields

$$\psi' = c_1\phi_1' + c_2\phi_2' \quad . \qquad (A.12)$$

We may solve for c_1 and c_2 in (A.11) and (A.12):

$$\psi\phi_2' - \psi'\phi_2 = c_1\underbrace{(\phi_1\phi_2' - \phi_2\phi_1')}_{D} \quad , \tag{A.13}$$

$$\psi'\phi_1 - \psi\phi_1' = c_2\underbrace{(\phi_1\phi_2' - \phi_2'\phi_1')}_{D} \quad . \tag{A.14}$$

Since the c coefficients are the quotients of Wronskians of (A.1), they are indeed constants, by (A.8). We may therefore use the argument at x' to for c_1 and c_2 in (A.11):

$$\psi(x) = c_1(x')\phi_1(x) + c_2(x')\phi_2(x) \quad . \tag{A.15}$$

Substituting from (A.13) and (A.14) in (A.15), we find

$$\begin{aligned}\psi(x) &= \frac{1}{D}[\psi(x')\phi_2'(x') - \psi'(x)\phi_2(x')]\phi_1(x) \\ &\quad + \frac{1}{D}[\psi'(x')\phi_1(x') - \psi(x')\phi_1'(x')]\phi_2(x) \quad .\end{aligned} \tag{A.16}$$

We may rearrange the terms in (A.16) to obtain an expression for $\psi(x)$ in terms of $\psi(x')$ and $\psi'(x')$:

$$\begin{aligned}\psi(x) &= \frac{1}{D}[\phi_1(x)\phi_2'(x') - \phi_2(x)\phi_1'(x')]\psi(x') \\ &\quad + \frac{1}{D}[\phi_2(x)\phi_1(x') - \phi_1(x)\phi_2(x')]\psi'(x') \\ &= b_{11}\psi(x') + b_{12}\psi'(x'), \text{ Q.E.D.}\end{aligned} \tag{A.17}$$

A similar argument will give the expressions for the matrix elements b_{21} and b_{22}.

A.2 Dispersion Relation

We now consider a different point of view, in which we express $\psi(x)$ in terms of its value at x', without regard to $\psi'(x')$. We again use (A.11), and write

$$\psi(x) = \lambda(x,x')\psi(x') \tag{A.18}$$

Using (A.18), and letting $\psi(x')$ also be of the form (A.11), there will be some matrix A with elements a_{ij}, such that

$$\phi_1(x) = a_{11}\phi_1(x') + a_{12}\phi_2(x') \tag{A.19}$$

and

$$\phi_2(x) = a_{21}\phi_1(x') + a_{12}\phi_2(x') \quad . \tag{A.20}$$

Equations (A.11) and (A.18)-(A.20) give us

$$\begin{aligned}\psi(x) &= \left(c_1 a_{11} + c_2 a_{21}\right)\phi_1(x') + \left(c_1 a_{12} + c_2 a_{22}\right)\phi_2(x') \\ &= \lambda\left[c_1\phi_1(x') + c_2\phi_2(x')\right] \quad .\end{aligned} \tag{A.21}$$

From (A.21) we obtain the matrix eigenvalue equation

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0 \quad , \tag{A.22}$$

or

$$\lambda^2 - (a_{11} + a_{22})\lambda + \underbrace{(a_{11}a_{22} - a_{12}\,a_{21})}_{\Delta} = 0 \quad . \tag{A.23}$$

We next show that $\Delta = 1$. Note however, that since $\Delta = 1$, we find

$$\lambda^2 - (a_{11} + a_{22})\lambda + 1 = 0 \quad , \tag{A.24}$$

or

$$T_r[A] = \lambda + \lambda^{-1} \qquad (A.25)$$

We now show that $\Delta = 1$. We refer to the (constant) Wronskian D. Using (A.19) and (A.20) we write

$$\begin{aligned} D &= \phi_1(x)\phi_2'(x) - \phi_1'(x)\phi_2(x) \\ &= [a_{11}\phi_1(x') + a_{12}\phi_2(x')]\,[a_{21}\phi_1'(x') + a_{22}\phi_2'(x')] \\ &\quad - [a_{11}\phi_1'(x') + a_{12}\phi_2'(x')]\,[a_{21}\phi_1(x') + a_{22}\phi_2(x')] \quad , \qquad (A.26) \end{aligned}$$

or

$$D = (a_{11}a_{22} - a_{12}a_{21})[\phi_1(x')\phi_2(x') - \phi_1'(x')\phi_2(x')] \quad . \qquad (A.27)$$

i.e.,

$$D = \Delta D \quad . \qquad (A.28)$$

Therefore

$$\Delta = 1 \quad . \qquad (A.29)$$

The results we have derived have depended on the form (A.1) for the wave equation, and in particular on the consequence (A.8). However, the expression (A.18) is most useful when ψ is periodic in x. This will be the case when f(x) is periodic, as we now show. We may construct a function A(x) such that

$$\psi(x) = A(x)\, e^{ikx} \quad . \qquad (A.30)$$

Substituting (A.29) in (A.1) we find

$$A'' + 2ikA' + [f(x) - k^2]\, A = 0 \quad . \qquad (A.31)$$

If f(x) is periodic with period d, then from (A.31) A must be also. It is often useful to rewrite (A.30) in another form. We let

$$x - x' = d \quad , \qquad (A.32)$$

and obtain

$$\psi = A(x' + nd)\exp\left[ikx' + iknd\right] \qquad (A.33)$$

$$= A_o(x')\exp\left[iknd\right] \quad . \qquad (A.34)$$

From (A.33) we see that

$$\lambda = e^{ikd} \qquad (A.35)$$

in (A.18). Using (A.35) in (A.25), we have the dispersion relation

$$T_r[A] = 2\cos kd \quad . \qquad (A.36)$$

If there is a first derivative in the wave equation, leading to (A.10) instead of (A-8) we would find

$$\exp\left[\Gamma(x') - \Gamma(x)\right] \quad , \qquad (A.37)$$

where

$$\Gamma = \int_o^r dx\ \gamma(x) \quad . \qquad (A.38)$$

Equations (A.11)-(A.23) would otherwise remain unchanged. Equation (A.24) would now become

$$\lambda^2 - (a_{11} + a_{22})\lambda + \exp\left[\Gamma(x') - \Gamma(x)\right] = 0 \qquad (A.39)$$

In the case of Equations (4-1) and (4-4) we have $\gamma\frac{d}{dx}\ln\varepsilon$, so that the third term in (A-39) becomes $\varepsilon(x)/\varepsilon(x')$.

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